



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 02:31 AM JST

PDB ID : 7CT5
EMDB ID : EMD-30460
Title : S protein of SARS-CoV-2 in complex bound with T-ACE2
Authors : Guo, L.; Bi, W.W.; Zhang, Y.Y.; Yan, R.H.; Li, Y.N.; Zhou, Q.; Dang, B.B.
Deposited on : 2020-08-18
Resolution : 4.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

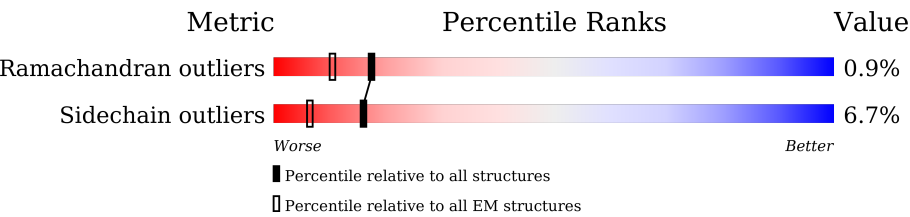
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









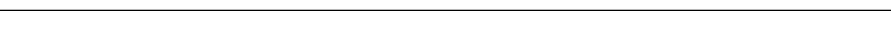
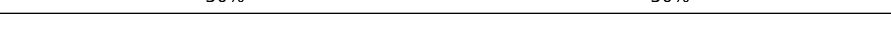
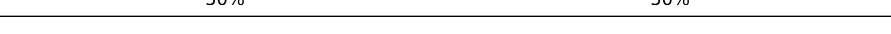
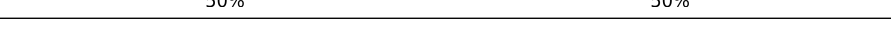
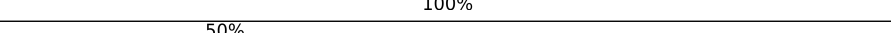
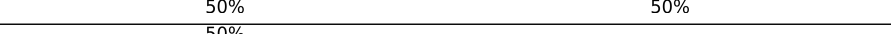
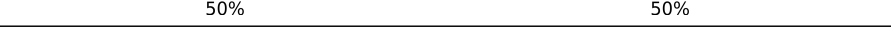

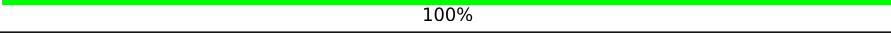

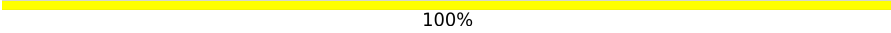
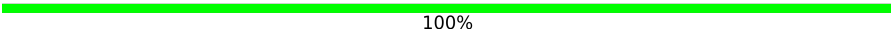


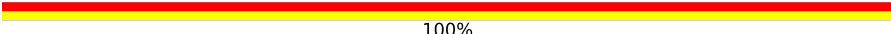


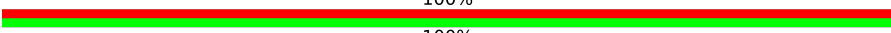

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1283	<div><div>9%</div><div>71%</div><div>7%</div><div>22%</div></div>
1	B	1283	<div><div>10%</div><div>72%</div><div>7%</div><div>22%</div></div>
1	C	1283	<div><div>6%</div><div>70%</div><div>7%</div><div>22%</div></div>
2	D	655	<div><div>79%</div><div>90%</div><div>9%</div></div>
2	E	655	<div><div>89%</div><div>90%</div><div>9%</div></div>
2	F	655	<div><div>62%</div><div>90%</div><div>9%</div></div>
3	G	2	<div><div>100%</div></div>
3	H	2	<div><div>50%</div><div>50%</div></div>
3	I	2	<div><div>50%</div><div>50%</div></div>

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Mol	Chain	Length	Quality of chain
3	J	2	 50%50%
3	K	2	 50%100%
3	L	2	 50%50%
3	M	2	 50%50%
3	N	2	 100%50%
3	O	2	 50%100%
3	P	2	 50%50%
3	Q	2	 50%50%
3	R	2	 50%50%
3	S	2	 100%
3	T	2	 50%50%
3	U	2	 50%50%
3	V	2	 50%50%
3	W	2	 100%
3	X	2	 100%50%
3	Y	2	 100%
3	Z	2	 100%
3	a	2	 100%100%
3	b	2	 100%100%
3	c	2	 100%100%
3	d	2	 100%100%
3	e	2	 50%50%
3	f	2	 100%100%
3	g	2	 100%100%
3	h	2	 100%100%

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Mol	Chain	Length	Quality of chain
3	i	2	<div><div>100%</div><div><div></div></div></div>
3	j	2	<div><div>100%</div><div><div></div></div></div>
3	k	2	<div><div>100%</div><div><div></div></div></div>
3	l	2	<div><div>100%</div><div><div></div></div></div>
3	m	2	<div><div>100%</div><div><div></div></div></div>
3	n	2	<div><div>100%</div><div><div></div></div></div>
3	o	2	<div><div>100%</div><div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39626 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1006	Total	C	N	O	S	0	0
			7863	5019	1308	1500	36		
1	B	1007	Total	C	N	O	S	0	0
			7870	5023	1310	1501	36		
1	C	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		
2	E	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		
2	F	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	GLY	-	expression tag	UNP Q9BYF1
D	617	SER	-	expression tag	UNP Q9BYF1
D	618	GLU	-	expression tag	UNP Q9BYF1
D	619	ALA	-	expression tag	UNP Q9BYF1
D	620	ALA	-	expression tag	UNP Q9BYF1
D	621	ALA	-	expression tag	UNP Q9BYF1
D	622	LYS	-	expression tag	UNP Q9BYF1
D	623	GLU	-	expression tag	UNP Q9BYF1
D	624	ALA	-	expression tag	UNP Q9BYF1
D	625	ALA	-	expression tag	UNP Q9BYF1
D	626	ALA	-	expression tag	UNP Q9BYF1
D	627	LYS	-	expression tag	UNP Q9BYF1
D	628	GLU	-	expression tag	UNP Q9BYF1
D	629	ALA	-	expression tag	UNP Q9BYF1
D	630	ALA	-	expression tag	UNP Q9BYF1
D	631	ALA	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	632	LYS	-	expression tag	UNP Q9BYF1
D	633	GLU	-	expression tag	UNP Q9BYF1
D	634	ALA	-	expression tag	UNP Q9BYF1
D	635	ALA	-	expression tag	UNP Q9BYF1
D	636	ALA	-	expression tag	UNP Q9BYF1
D	637	LYS	-	expression tag	UNP Q9BYF1
D	638	GLU	-	expression tag	UNP Q9BYF1
D	639	ALA	-	expression tag	UNP Q9BYF1
D	640	ALA	-	expression tag	UNP Q9BYF1
D	641	ALA	-	expression tag	UNP Q9BYF1
D	642	LYS	-	expression tag	UNP Q9BYF1
D	643	GLY	-	expression tag	UNP Q9BYF1
D	644	SER	-	expression tag	UNP Q9BYF1
D	645	GLY	-	expression tag	UNP Q9BYF1
D	646	TYR	-	expression tag	UNP Q9BYF1
D	647	ILE	-	expression tag	UNP Q9BYF1
D	648	PRO	-	expression tag	UNP Q9BYF1
D	649	GLU	-	expression tag	UNP Q9BYF1
D	650	ALA	-	expression tag	UNP Q9BYF1
D	651	PRO	-	expression tag	UNP Q9BYF1
D	652	ARG	-	expression tag	UNP Q9BYF1
D	653	ASP	-	expression tag	UNP Q9BYF1
D	654	GLY	-	expression tag	UNP Q9BYF1
D	655	GLN	-	expression tag	UNP Q9BYF1
D	656	ALA	-	expression tag	UNP Q9BYF1
D	657	TYR	-	expression tag	UNP Q9BYF1
D	658	VAL	-	expression tag	UNP Q9BYF1
D	659	ARG	-	expression tag	UNP Q9BYF1
D	660	LYS	-	expression tag	UNP Q9BYF1
D	661	ASP	-	expression tag	UNP Q9BYF1
D	662	GLY	-	expression tag	UNP Q9BYF1
D	663	GLU	-	expression tag	UNP Q9BYF1
D	664	TRP	-	expression tag	UNP Q9BYF1
D	665	VAL	-	expression tag	UNP Q9BYF1
D	666	LEU	-	expression tag	UNP Q9BYF1
D	667	LEU	-	expression tag	UNP Q9BYF1
D	668	SER	-	expression tag	UNP Q9BYF1
D	669	THR	-	expression tag	UNP Q9BYF1
D	670	PHE	-	expression tag	UNP Q9BYF1
D	671	LEU	-	expression tag	UNP Q9BYF1
D	672	GLY	-	expression tag	UNP Q9BYF1
D	673	SER	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	616	GLY	-	expression tag	UNP Q9BYF1
E	617	SER	-	expression tag	UNP Q9BYF1
E	618	GLU	-	expression tag	UNP Q9BYF1
E	619	ALA	-	expression tag	UNP Q9BYF1
E	620	ALA	-	expression tag	UNP Q9BYF1
E	621	ALA	-	expression tag	UNP Q9BYF1
E	622	LYS	-	expression tag	UNP Q9BYF1
E	623	GLU	-	expression tag	UNP Q9BYF1
E	624	ALA	-	expression tag	UNP Q9BYF1
E	625	ALA	-	expression tag	UNP Q9BYF1
E	626	ALA	-	expression tag	UNP Q9BYF1
E	627	LYS	-	expression tag	UNP Q9BYF1
E	628	GLU	-	expression tag	UNP Q9BYF1
E	629	ALA	-	expression tag	UNP Q9BYF1
E	630	ALA	-	expression tag	UNP Q9BYF1
E	631	ALA	-	expression tag	UNP Q9BYF1
E	632	LYS	-	expression tag	UNP Q9BYF1
E	633	GLU	-	expression tag	UNP Q9BYF1
E	634	ALA	-	expression tag	UNP Q9BYF1
E	635	ALA	-	expression tag	UNP Q9BYF1
E	636	ALA	-	expression tag	UNP Q9BYF1
E	637	LYS	-	expression tag	UNP Q9BYF1
E	638	GLU	-	expression tag	UNP Q9BYF1
E	639	ALA	-	expression tag	UNP Q9BYF1
E	640	ALA	-	expression tag	UNP Q9BYF1
E	641	ALA	-	expression tag	UNP Q9BYF1
E	642	LYS	-	expression tag	UNP Q9BYF1
E	643	GLY	-	expression tag	UNP Q9BYF1
E	644	SER	-	expression tag	UNP Q9BYF1
E	645	GLY	-	expression tag	UNP Q9BYF1
E	646	TYR	-	expression tag	UNP Q9BYF1
E	647	ILE	-	expression tag	UNP Q9BYF1
E	648	PRO	-	expression tag	UNP Q9BYF1
E	649	GLU	-	expression tag	UNP Q9BYF1
E	650	ALA	-	expression tag	UNP Q9BYF1
E	651	PRO	-	expression tag	UNP Q9BYF1
E	652	ARG	-	expression tag	UNP Q9BYF1
E	653	ASP	-	expression tag	UNP Q9BYF1
E	654	GLY	-	expression tag	UNP Q9BYF1
E	655	GLN	-	expression tag	UNP Q9BYF1
E	656	ALA	-	expression tag	UNP Q9BYF1
E	657	TYR	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	658	VAL	-	expression tag	UNP Q9BYF1
E	659	ARG	-	expression tag	UNP Q9BYF1
E	660	LYS	-	expression tag	UNP Q9BYF1
E	661	ASP	-	expression tag	UNP Q9BYF1
E	662	GLY	-	expression tag	UNP Q9BYF1
E	663	GLU	-	expression tag	UNP Q9BYF1
E	664	TRP	-	expression tag	UNP Q9BYF1
E	665	VAL	-	expression tag	UNP Q9BYF1
E	666	LEU	-	expression tag	UNP Q9BYF1
E	667	LEU	-	expression tag	UNP Q9BYF1
E	668	SER	-	expression tag	UNP Q9BYF1
E	669	THR	-	expression tag	UNP Q9BYF1
E	670	PHE	-	expression tag	UNP Q9BYF1
E	671	LEU	-	expression tag	UNP Q9BYF1
E	672	GLY	-	expression tag	UNP Q9BYF1
E	673	SER	-	expression tag	UNP Q9BYF1
F	616	GLY	-	expression tag	UNP Q9BYF1
F	617	SER	-	expression tag	UNP Q9BYF1
F	618	GLU	-	expression tag	UNP Q9BYF1
F	619	ALA	-	expression tag	UNP Q9BYF1
F	620	ALA	-	expression tag	UNP Q9BYF1
F	621	ALA	-	expression tag	UNP Q9BYF1
F	622	LYS	-	expression tag	UNP Q9BYF1
F	623	GLU	-	expression tag	UNP Q9BYF1
F	624	ALA	-	expression tag	UNP Q9BYF1
F	625	ALA	-	expression tag	UNP Q9BYF1
F	626	ALA	-	expression tag	UNP Q9BYF1
F	627	LYS	-	expression tag	UNP Q9BYF1
F	628	GLU	-	expression tag	UNP Q9BYF1
F	629	ALA	-	expression tag	UNP Q9BYF1
F	630	ALA	-	expression tag	UNP Q9BYF1
F	631	ALA	-	expression tag	UNP Q9BYF1
F	632	LYS	-	expression tag	UNP Q9BYF1
F	633	GLU	-	expression tag	UNP Q9BYF1
F	634	ALA	-	expression tag	UNP Q9BYF1
F	635	ALA	-	expression tag	UNP Q9BYF1
F	636	ALA	-	expression tag	UNP Q9BYF1
F	637	LYS	-	expression tag	UNP Q9BYF1
F	638	GLU	-	expression tag	UNP Q9BYF1
F	639	ALA	-	expression tag	UNP Q9BYF1
F	640	ALA	-	expression tag	UNP Q9BYF1
F	641	ALA	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	642	LYS	-	expression tag	UNP Q9BYF1
F	643	GLY	-	expression tag	UNP Q9BYF1
F	644	SER	-	expression tag	UNP Q9BYF1
F	645	GLY	-	expression tag	UNP Q9BYF1
F	646	TYR	-	expression tag	UNP Q9BYF1
F	647	ILE	-	expression tag	UNP Q9BYF1
F	648	PRO	-	expression tag	UNP Q9BYF1
F	649	GLU	-	expression tag	UNP Q9BYF1
F	650	ALA	-	expression tag	UNP Q9BYF1
F	651	PRO	-	expression tag	UNP Q9BYF1
F	652	ARG	-	expression tag	UNP Q9BYF1
F	653	ASP	-	expression tag	UNP Q9BYF1
F	654	GLY	-	expression tag	UNP Q9BYF1
F	655	GLN	-	expression tag	UNP Q9BYF1
F	656	ALA	-	expression tag	UNP Q9BYF1
F	657	TYR	-	expression tag	UNP Q9BYF1
F	658	VAL	-	expression tag	UNP Q9BYF1
F	659	ARG	-	expression tag	UNP Q9BYF1
F	660	LYS	-	expression tag	UNP Q9BYF1
F	661	ASP	-	expression tag	UNP Q9BYF1
F	662	GLY	-	expression tag	UNP Q9BYF1
F	663	GLU	-	expression tag	UNP Q9BYF1
F	664	TRP	-	expression tag	UNP Q9BYF1
F	665	VAL	-	expression tag	UNP Q9BYF1
F	666	LEU	-	expression tag	UNP Q9BYF1
F	667	LEU	-	expression tag	UNP Q9BYF1
F	668	SER	-	expression tag	UNP Q9BYF1
F	669	THR	-	expression tag	UNP Q9BYF1
F	670	PHE	-	expression tag	UNP Q9BYF1
F	671	LEU	-	expression tag	UNP Q9BYF1
F	672	GLY	-	expression tag	UNP Q9BYF1
F	673	SER	-	expression tag	UNP Q9BYF1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	j	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		
3	l	2	Total	C	N	O	0	0
			28	16	2	10		
3	m	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		
3	o	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



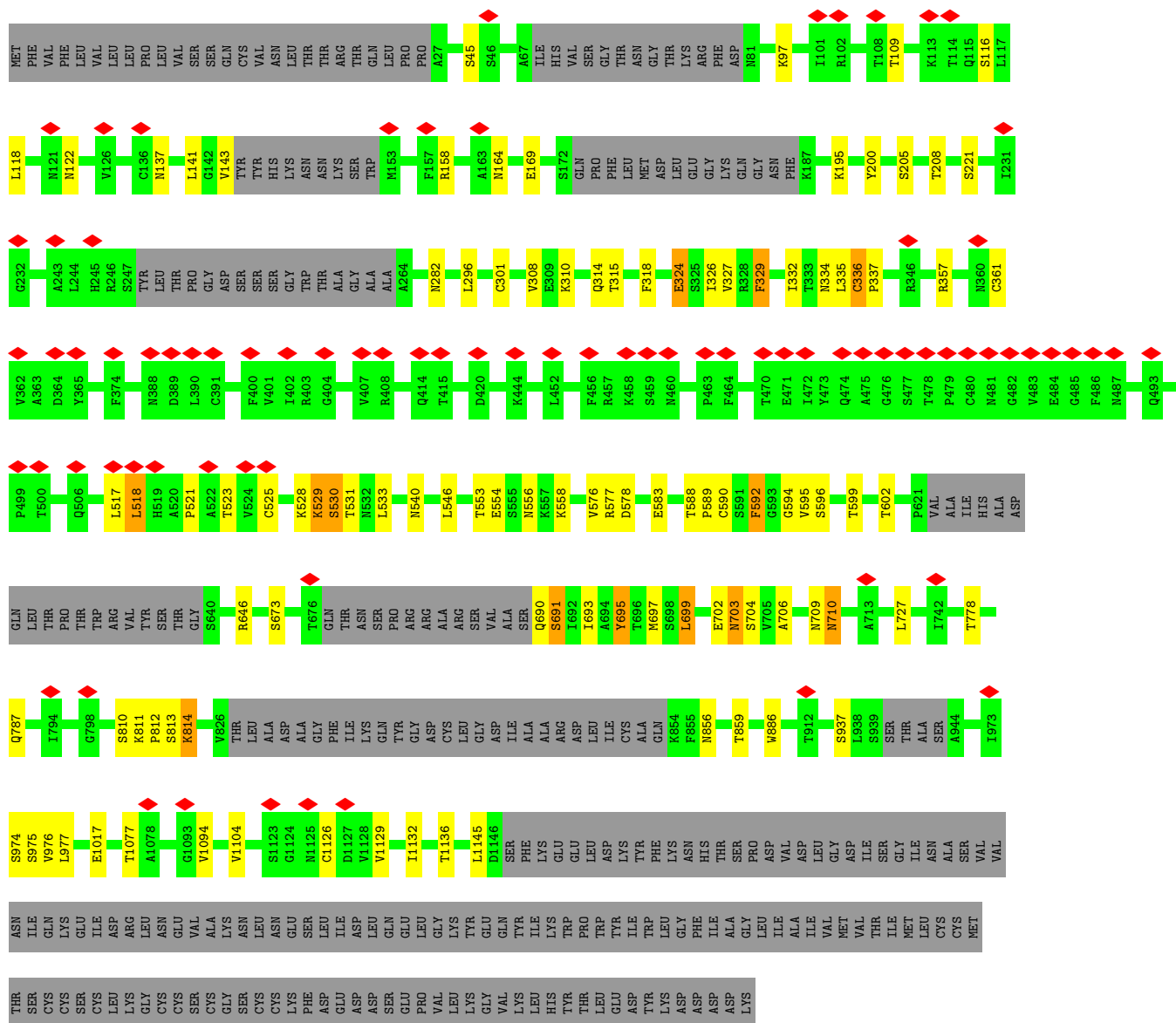
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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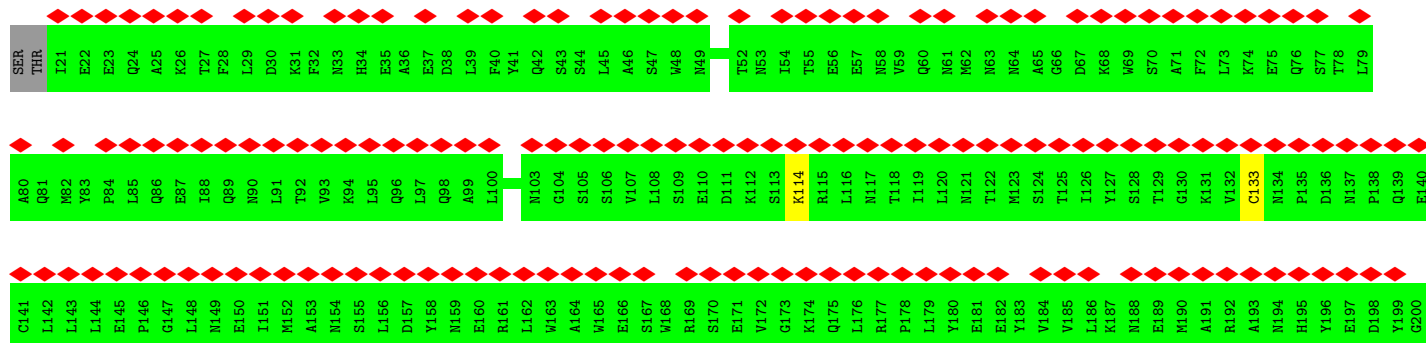
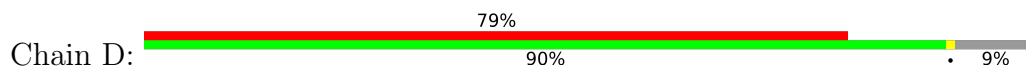
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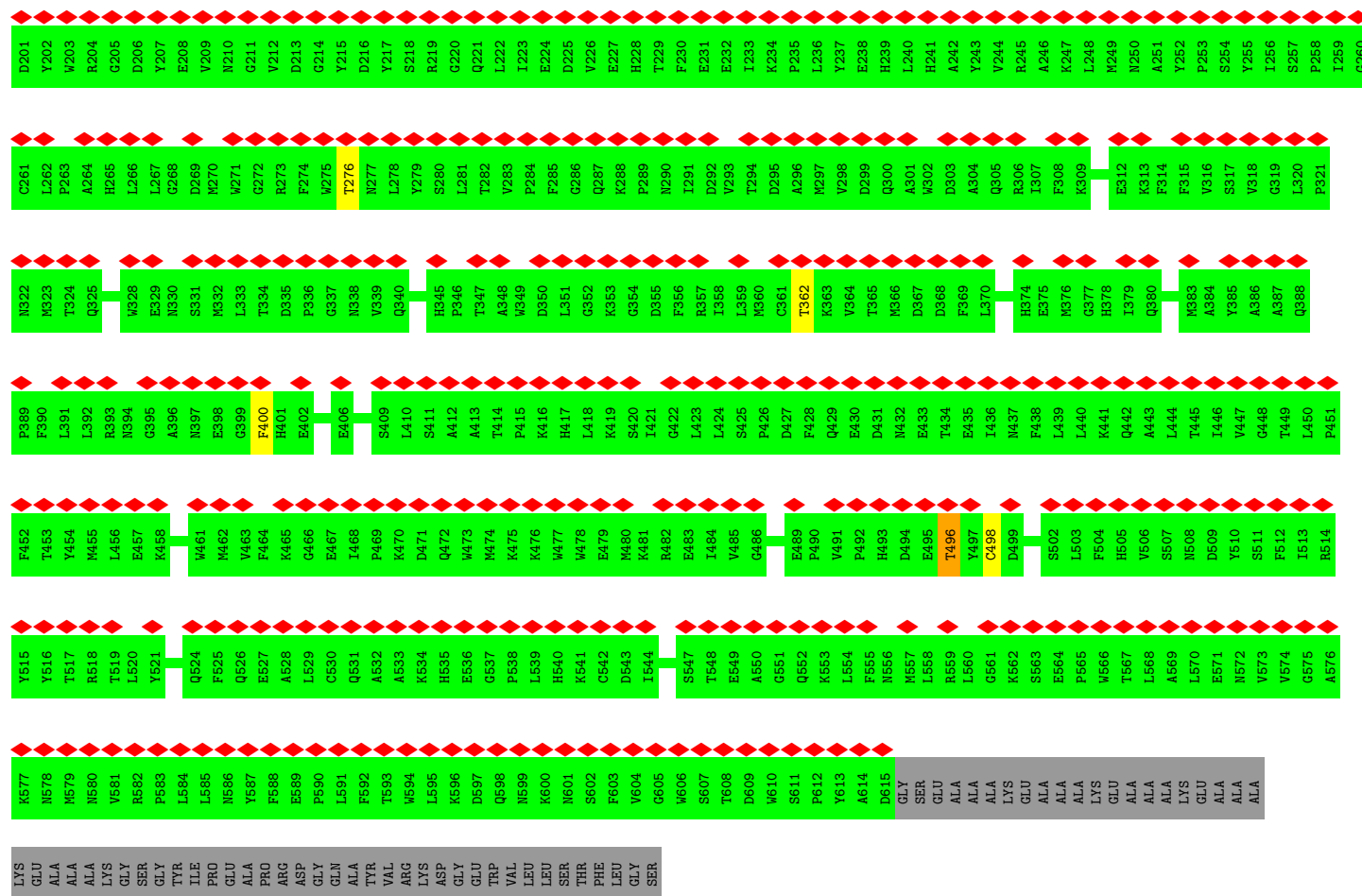
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	E	1	Total 14	C 8	N 1	O 5	0
4	F	1	Total 14	C 8	N 1	O 5	0

Chain C:  6% 70% 7% 22%

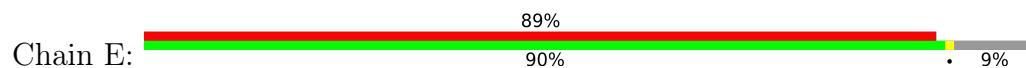


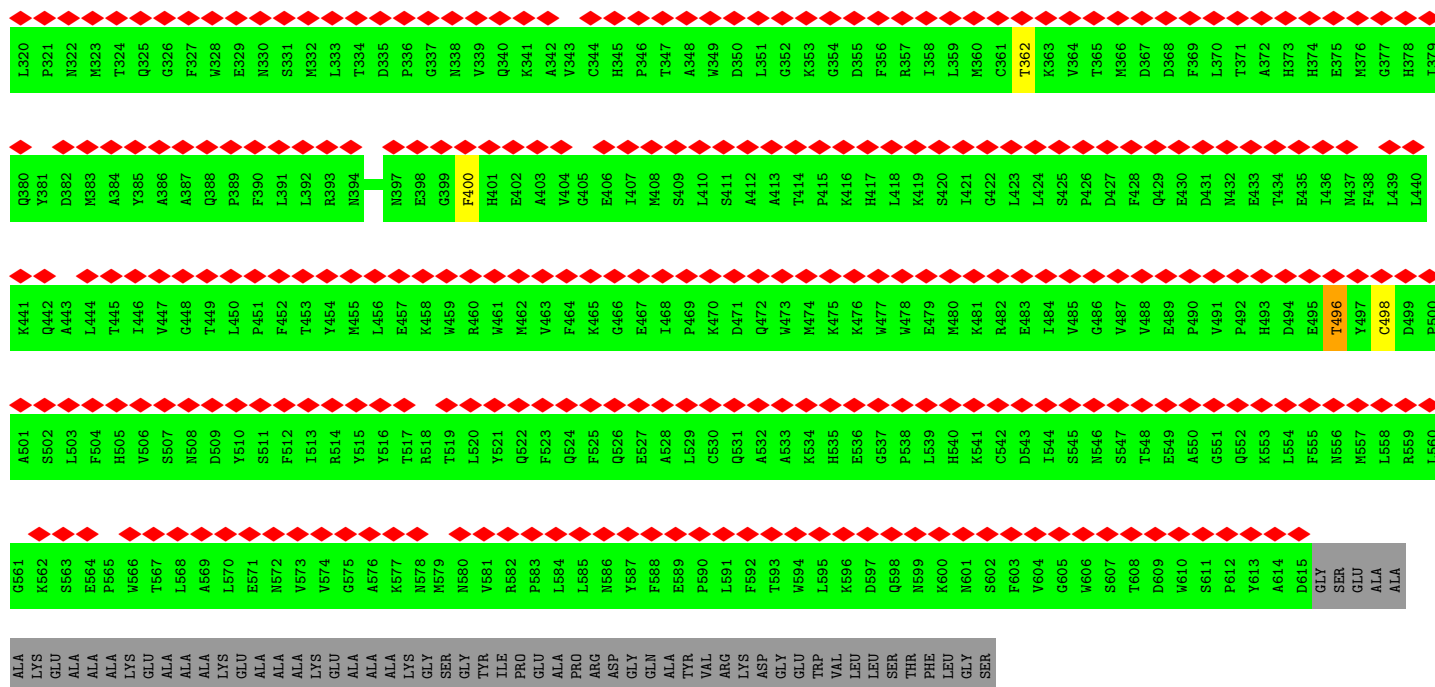
• Molecule 2: Angiotensin-converting enzyme 2



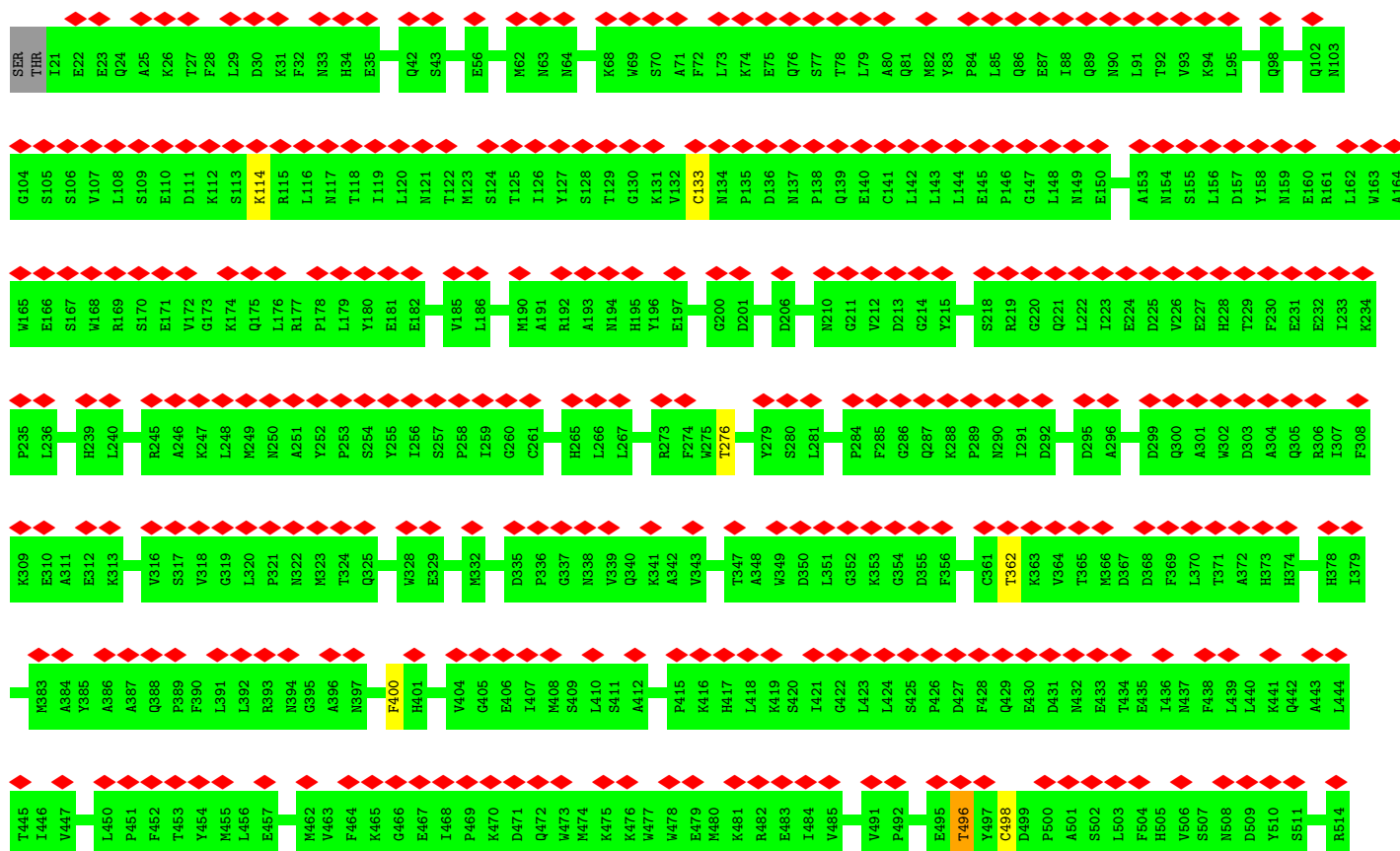
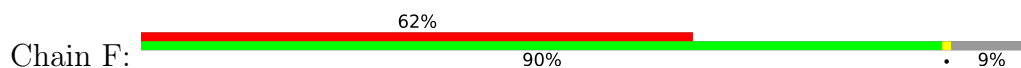


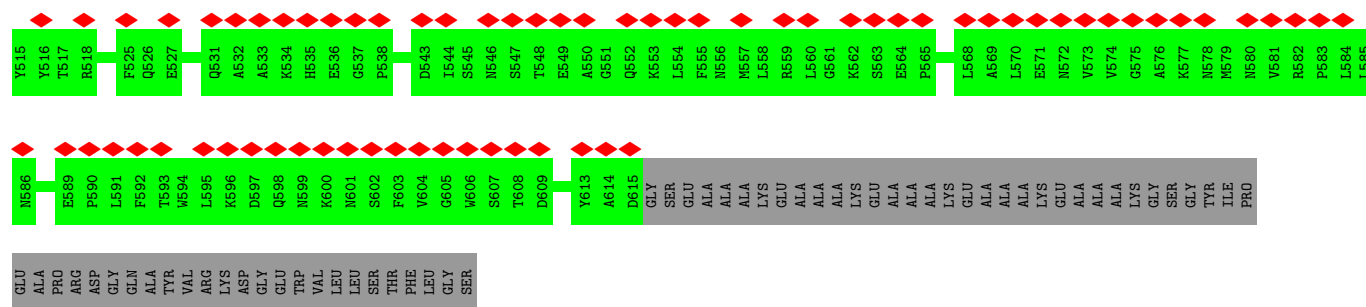
• Molecule 2: Angiotensin-converting enzyme 2





• Molecule 2: Angiotensin-converting enzyme 2





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 100% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100% 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/8039	0.56	0/10936
1	B	0.51	0/8045	0.56	0/10942
1	C	0.50	0/8042	0.54	0/10939
2	D	0.39	0/4994	0.54	0/6785
2	E	0.39	0/4994	0.54	0/6785
2	F	0.39	0/4994	0.54	0/6785
All	All	0.47	0/39108	0.55	0/53172

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	988/1283 (77%)	874 (88%)	108 (11%)	6 (1%)	22	58
1	B	989/1283 (77%)	874 (88%)	109 (11%)	6 (1%)	22	58
1	C	988/1283 (77%)	849 (86%)	109 (11%)	30 (3%)	3	27
2	D	593/655 (90%)	560 (94%)	32 (5%)	1 (0%)	44	76
2	E	593/655 (90%)	560 (94%)	32 (5%)	1 (0%)	44	76
2	F	593/655 (90%)	560 (94%)	32 (5%)	1 (0%)	44	76
All	All	4744/5814 (82%)	4277 (90%)	422 (9%)	45 (1%)	17	49

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	983	ARG
1	C	332	ILE
1	C	518	LEU
1	C	529	LYS
1	C	530	SER
1	C	531	THR
1	C	589	PRO
1	C	702	GLU
1	C	703	ASN
1	C	706	ALA
1	C	710	ASN
1	C	814	LYS
1	A	333	THR
1	A	521	PRO
1	B	331	ASN
1	B	518	LEU
1	B	528	LYS
1	C	324	GLU
1	C	327	VAL
1	C	695	TYR
1	C	699	LEU
1	C	810	SER
2	D	496	THR
2	E	496	THR
2	F	496	THR
1	C	337	PRO
1	C	596	SER
1	C	704	SER
1	C	709	ASN
1	A	336	CYS

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Mol	Chain	Res	Type
1	A	982	SER
1	B	332	ILE
1	B	524	VAL
1	C	329	PHE
1	C	521	PRO
1	C	592	PHE
1	C	691	SER
1	C	813	SER
1	B	333	THR
1	C	812	PRO
1	A	590	CYS
1	C	336	CYS
1	C	811	LYS
1	C	594	GLY
1	C	595	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	881/1122 (78%)	793 (90%)	88 (10%)	6	23
1	B	881/1122 (78%)	796 (90%)	85 (10%)	7	24
1	C	881/1122 (78%)	794 (90%)	87 (10%)	6	23
2	D	525/562 (93%)	518 (99%)	7 (1%)	65	77
2	E	525/562 (93%)	518 (99%)	7 (1%)	65	77
2	F	525/562 (93%)	518 (99%)	7 (1%)	65	77
All	All	4218/5052 (84%)	3937 (93%)	281 (7%)	16	36

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	97	LYS
1	A	109	THR

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Mol	Chain	Res	Type
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	137	ASN
1	A	141	LEU
1	A	143	VAL
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	282	ASN
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	318	PHE
1	A	324	GLU
1	A	334	ASN
1	A	335	LEU
1	A	336	CYS
1	A	338	PHE
1	A	357	ARG
1	A	525	CYS
1	A	528	LYS
1	A	529	LYS
1	A	533	LEU
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	558	LYS
1	A	576	VAL
1	A	583	GLU
1	A	588	THR
1	A	590	CYS
1	A	591	SER
1	A	599	THR

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Mol	Chain	Res	Type
1	A	602	THR
1	A	646	ARG
1	A	673	SER
1	A	698	SER
1	A	703	ASN
1	A	722	VAL
1	A	727	LEU
1	A	729	VAL
1	A	738	CYS
1	A	746	SER
1	A	773	GLU
1	A	785	VAL
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU
1	A	929	SER
1	A	937	SER
1	A	939	SER
1	A	951	VAL
1	A	967	SER
1	A	983	ARG
1	A	985	ASP
1	A	988	GLU
1	A	994	ASP
1	A	1005	GLN
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1123	SER
1	A	1125	ASN
1	A	1132	ILE
1	A	1141	LEU
1	A	1142	GLN

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Mol	Chain	Res	Type
1	A	1144	GLU
1	B	45	SER
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	137	ASN
1	B	141	LEU
1	B	143	VAL
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	195	LYS
1	B	197	ILE
1	B	200	TYR
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	282	ASN
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL
1	B	314	GLN
1	B	315	THR
1	B	318	PHE
1	B	324	GLU
1	B	328	ARG
1	B	335	LEU
1	B	357	ARG
1	B	518	LEU
1	B	523	THR
1	B	525	CYS
1	B	528	LYS
1	B	529	LYS
1	B	531	THR
1	B	532	ASN
1	B	533	LEU
1	B	537	LYS
1	B	540	ASN
1	B	546	LEU
1	B	553	THR

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Mol	Chain	Res	Type
1	B	554	GLU
1	B	556	ASN
1	B	558	LYS
1	B	576	VAL
1	B	583	GLU
1	B	597	VAL
1	B	606	ASN
1	B	607	GLN
1	B	614	ASP
1	B	615	VAL
1	B	617	CYS
1	B	640	SER
1	B	649	CYS
1	B	676	THR
1	B	704	SER
1	B	710	ASN
1	B	746	SER
1	B	779	GLN
1	B	786	LYS
1	B	787	GLN
1	B	791	THR
1	B	808	ASP
1	B	854	LYS
1	B	855	PHE
1	B	856	ASN
1	B	868	GLU
1	B	878	LEU
1	B	912	THR
1	B	916	LEU
1	B	935	GLN
1	B	964	LYS
1	B	968	SER
1	B	969	ASN
1	B	974	SER
1	B	976	VAL
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE

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Mol	Chain	Res	Type
1	B	1126	CYS
1	B	1141	LEU
1	C	45	SER
1	C	97	LYS
1	C	109	THR
1	C	116	SER
1	C	118	LEU
1	C	122	ASN
1	C	137	ASN
1	C	141	LEU
1	C	143	VAL
1	C	158	ARG
1	C	164	ASN
1	C	169	GLU
1	C	195	LYS
1	C	200	TYR
1	C	205	SER
1	C	208	THR
1	C	221	SER
1	C	282	ASN
1	C	296	LEU
1	C	301	CYS
1	C	308	VAL
1	C	310	LYS
1	C	314	GLN
1	C	315	THR
1	C	318	PHE
1	C	324	GLU
1	C	326	ILE
1	C	329	PHE
1	C	334	ASN
1	C	335	LEU
1	C	336	CYS
1	C	357	ARG
1	C	361	CYS
1	C	517	LEU
1	C	518	LEU
1	C	523	THR
1	C	525	CYS
1	C	528	LYS
1	C	529	LYS
1	C	530	SER

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Mol	Chain	Res	Type
1	C	533	LEU
1	C	540	ASN
1	C	546	LEU
1	C	553	THR
1	C	554	GLU
1	C	556	ASN
1	C	558	LYS
1	C	576	VAL
1	C	577	ARG
1	C	578	ASP
1	C	583	GLU
1	C	588	THR
1	C	590	CYS
1	C	592	PHE
1	C	599	THR
1	C	602	THR
1	C	646	ARG
1	C	673	SER
1	C	690	GLN
1	C	691	SER
1	C	693	ILE
1	C	695	TYR
1	C	697	MET
1	C	699	LEU
1	C	703	ASN
1	C	710	ASN
1	C	727	LEU
1	C	778	THR
1	C	787	GLN
1	C	814	LYS
1	C	856	ASN
1	C	859	THR
1	C	886	TRP
1	C	937	SER
1	C	974	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1017	GLU
1	C	1077	THR
1	C	1094	VAL
1	C	1104	VAL

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Mol	Chain	Res	Type
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU
2	D	114	LYS
2	D	133	CYS
2	D	276	THR
2	D	362	THR
2	D	400	PHE
2	D	496	THR
2	D	498	CYS
2	E	114	LYS
2	E	133	CYS
2	E	276	THR
2	E	362	THR
2	E	400	PHE
2	E	496	THR
2	E	498	CYS
2	F	114	LYS
2	F	133	CYS
2	F	276	THR
2	F	362	THR
2	F	400	PHE
2	F	496	THR
2	F	498	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	239	GLN
1	A	360	ASN
1	A	414	GLN
1	A	422	ASN
1	A	450	ASN
1	A	460	ASN
1	A	493	GLN
1	A	540	ASN
1	A	556	ASN

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Mol	Chain	Res	Type
1	A	644	GLN
1	A	655	HIS
1	A	658	ASN
1	A	690	GLN
1	A	703	ASN
1	A	762	GLN
1	A	787	GLN
1	A	856	ASN
1	A	901	GLN
1	A	914	ASN
1	A	919	ASN
1	A	926	GLN
1	A	955	ASN
1	A	960	ASN
1	A	969	ASN
1	A	992	GLN
1	A	1125	ASN
1	A	1142	GLN
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	239	GLN
1	B	317	ASN
1	B	334	ASN
1	B	360	ASN
1	B	414	GLN
1	B	422	ASN
1	B	450	ASN
1	B	460	ASN
1	B	493	GLN
1	B	540	ASN
1	B	556	ASN
1	B	606	ASN
1	B	607	GLN
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	920	GLN
1	B	926	GLN
1	B	992	GLN

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Mol	Chain	Res	Type
1	B	1054	GLN
1	C	134	GLN
1	C	137	ASN
1	C	188	ASN
1	C	239	GLN
1	C	334	ASN
1	C	360	ASN
1	C	414	GLN
1	C	422	ASN
1	C	450	ASN
1	C	460	ASN
1	C	493	GLN
1	C	540	ASN
1	C	556	ASN
1	C	613	GLN
1	C	644	GLN
1	C	658	ASN
1	C	690	GLN
1	C	703	ASN
1	C	784	GLN
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	926	GLN
1	C	935	GLN
1	C	969	ASN
1	C	992	GLN
1	C	1010	GLN
1	C	1071	GLN
1	C	1101	HIS
1	C	1106	GLN
2	D	63	ASN
2	D	81	GLN
2	D	134	ASN
2	D	139	GLN
2	D	330	ASN
2	D	340	GLN
2	D	394	ASN
2	D	417	HIS
2	D	522	GLN
2	D	540	HIS

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Mol	Chain	Res	Type
2	D	552	GLN
2	D	556	ASN
2	D	586	ASN
2	E	63	ASN
2	E	81	GLN
2	E	134	ASN
2	E	139	GLN
2	E	340	GLN
2	E	394	ASN
2	E	417	HIS
2	E	522	GLN
2	E	540	HIS
2	E	552	GLN
2	E	556	ASN
2	E	586	ASN
2	F	63	ASN
2	F	81	GLN
2	F	134	ASN
2	F	139	GLN
2	F	330	ASN
2	F	340	GLN
2	F	394	ASN
2	F	417	HIS
2	F	522	GLN
2	F	540	HIS
2	F	552	GLN
2	F	556	ASN
2	F	586	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

70 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	G	1	1,3	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	1.16	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.31	0	17,19,21	0.71	0
3	NAG	H	2	3	14,14,15	0.51	0	17,19,21	0.64	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.35	0	17,19,21	0.62	1 (5%)
3	NAG	I	2	3	14,14,15	0.52	0	17,19,21	0.46	0
3	NAG	J	1	1,3	14,14,15	0.38	0	17,19,21	0.74	0
3	NAG	J	2	3	14,14,15	0.30	0	17,19,21	1.31	2 (11%)
3	NAG	K	1	1,3	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
3	NAG	K	2	3	14,14,15	0.39	0	17,19,21	1.38	3 (17%)
3	NAG	L	1	1,3	14,14,15	0.69	1 (7%)	17,19,21	0.67	0
3	NAG	L	2	3	14,14,15	0.28	0	17,19,21	0.64	0
3	NAG	M	1	1,3	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
3	NAG	M	2	3	14,14,15	0.16	0	17,19,21	0.45	0
3	NAG	N	1	1,3	14,14,15	0.31	0	17,19,21	0.71	0
3	NAG	N	2	3	14,14,15	0.50	0	17,19,21	0.63	1 (5%)
3	NAG	O	1	1,3	14,14,15	0.33	0	17,19,21	0.41	0
3	NAG	O	2	3	14,14,15	0.39	0	17,19,21	0.36	0
3	NAG	P	1	1,3	14,14,15	0.34	0	17,19,21	1.10	1 (5%)
3	NAG	P	2	3	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	Q	1	1,3	14,14,15	0.31	0	17,19,21	0.69	1 (5%)
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	R	1	1,3	14,14,15	0.77	1 (7%)	17,19,21	0.90	1 (5%)
3	NAG	R	2	3	14,14,15	0.30	0	17,19,21	0.66	0
3	NAG	S	1	1,3	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	S	2	3	14,14,15	0.28	0	17,19,21	0.38	0
3	NAG	T	1	1,3	14,14,15	0.30	0	17,19,21	0.72	0
3	NAG	T	2	3	14,14,15	0.52	0	17,19,21	0.64	1 (5%)
3	NAG	U	1	1,3	14,14,15	0.23	0	17,19,21	1.35	1 (5%)
3	NAG	U	2	3	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	V	1	1,3	14,14,15	0.55	0	17,19,21	0.71	1 (5%)
3	NAG	V	2	3	14,14,15	0.40	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	W	1	1,3	14,14,15	0.38	0	17,19,21	0.42	0
3	NAG	W	2	3	14,14,15	0.26	0	17,19,21	0.72	0
3	NAG	X	1	1,3	14,14,15	0.37	0	17,19,21	0.47	0
3	NAG	X	2	3	14,14,15	0.55	0	17,19,21	1.32	1 (5%)
3	NAG	Y	1	1,3	14,14,15	0.67	1 (7%)	17,19,21	0.44	0
3	NAG	Y	2	3	14,14,15	0.30	0	17,19,21	1.35	2 (11%)
3	NAG	Z	1	1,3	14,14,15	0.43	0	17,19,21	0.43	0
3	NAG	Z	2	3	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	a	1	2,3	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	a	2	3	14,14,15	0.59	0	17,19,21	0.45	0
3	NAG	b	1	2,3	14,14,15	0.47	0	17,19,21	0.60	0
3	NAG	b	2	3	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	c	1	2,3	14,14,15	0.60	1 (7%)	17,19,21	1.29	2 (11%)
3	NAG	c	2	3	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
3	NAG	d	1	2,3	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	d	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	e	1	2,3	14,14,15	0.66	1 (7%)	17,19,21	0.83	0
3	NAG	e	2	3	14,14,15	0.25	0	17,19,21	0.55	0
3	NAG	f	1	2,3	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	f	2	3	14,14,15	0.59	0	17,19,21	0.46	0
3	NAG	g	1	2,3	14,14,15	0.48	0	17,19,21	0.60	0
3	NAG	g	2	3	14,14,15	0.27	0	17,19,21	0.58	0
3	NAG	h	1	2,3	14,14,15	0.61	1 (7%)	17,19,21	1.29	2 (11%)
3	NAG	h	2	3	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
3	NAG	i	1	2,3	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	i	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	j	1	2,3	14,14,15	0.66	1 (7%)	17,19,21	0.83	0
3	NAG	j	2	3	14,14,15	0.24	0	17,19,21	0.55	0
3	NAG	k	1	2,3	14,14,15	0.34	0	17,19,21	0.61	0
3	NAG	k	2	3	14,14,15	0.57	0	17,19,21	0.44	0
3	NAG	l	1	2,3	14,14,15	0.47	0	17,19,21	0.61	0
3	NAG	l	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	m	1	2,3	14,14,15	0.61	1 (7%)	17,19,21	1.28	2 (11%)
3	NAG	m	2	3	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
3	NAG	n	1	2,3	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	n	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	o	1	2,3	14,14,15	0.65	1 (7%)	17,19,21	0.83	0
3	NAG	o	2	3	14,14,15	0.23	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	5/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	5/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	4/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	NAG	a	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	NAG	c	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	NAG	e	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	NAG	j	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1
3	NAG	k	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	k	2	3	-	2/6/23/26	0/1/1/1
3	NAG	l	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	NAG	m	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	2/6/23/26	0/1/1/1
3	NAG	n	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	2/6/23/26	0/1/1/1
3	NAG	o	1	2,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	o	2	3	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C1	-2.80	1.39	1.43
3	L	1	NAG	O5-C1	-2.51	1.39	1.43
3	K	1	NAG	O5-C1	-2.35	1.40	1.43
3	Y	1	NAG	O5-C1	-2.27	1.40	1.43
3	j	1	NAG	O5-C1	-2.25	1.40	1.43
3	e	1	NAG	O5-C1	-2.22	1.40	1.43
3	o	1	NAG	O5-C1	-2.22	1.40	1.43
3	m	1	NAG	O5-C1	2.04	1.47	1.43
3	h	1	NAG	O5-C1	2.03	1.47	1.43
3	c	1	NAG	O5-C1	2.01	1.46	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1	NAG	C2-N2-C7	4.61	129.47	122.90
3	h	1	NAG	C1-O5-C5	4.43	118.19	112.19
3	c	1	NAG	C1-O5-C5	4.42	118.19	112.19
3	m	1	NAG	C1-O5-C5	4.41	118.16	112.19
3	Y	2	NAG	C2-N2-C7	4.36	129.11	122.90
3	X	2	NAG	C2-N2-C7	4.35	129.09	122.90
3	J	2	NAG	C2-N2-C7	4.29	129.01	122.90
3	K	2	NAG	C2-N2-C7	4.27	128.99	122.90
3	P	1	NAG	C1-O5-C5	3.22	116.56	112.19
3	m	2	NAG	C1-O5-C5	2.59	115.71	112.19
3	h	2	NAG	C1-O5-C5	2.59	115.70	112.19
3	c	2	NAG	C1-O5-C5	2.59	115.70	112.19
3	K	2	NAG	C1-C2-N2	2.47	114.70	110.49
3	G	1	NAG	C8-C7-N2	2.40	120.16	116.10
3	R	1	NAG	O4-C4-C3	-2.36	104.90	110.35
3	G	2	NAG	C8-C7-N2	2.35	120.08	116.10
3	Y	2	NAG	C1-C2-N2	2.32	114.44	110.49
3	c	1	NAG	O4-C4-C5	2.28	114.95	109.30
3	Q	1	NAG	C1-O5-C5	2.27	115.27	112.19
3	m	1	NAG	O4-C4-C5	2.27	114.93	109.30
3	h	1	NAG	O4-C4-C5	2.27	114.93	109.30
3	J	2	NAG	C1-C2-N2	2.27	114.36	110.49
3	M	1	NAG	C1-O5-C5	2.25	115.24	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	1	NAG	C1-O5-C5	2.25	115.23	112.19
3	T	2	NAG	C1-O5-C5	2.14	115.09	112.19
3	N	2	NAG	C1-O5-C5	2.12	115.07	112.19
3	H	2	NAG	C1-O5-C5	2.12	115.07	112.19
3	K	2	NAG	C1-O5-C5	2.04	114.96	112.19
3	I	1	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	f	1	NAG	O5-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
3	n	2	NAG	C4-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	l	2	NAG	C4-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	X	2	NAG	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	m	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	f	1	NAG	C4-C5-C6-O6
3	k	1	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	k	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	X	2	NAG	C8-C7-N2-C2
3	X	2	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
3	S	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	m	2	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
3	n	2	NAG	O5-C5-C6-O6
3	c	1	NAG	C4-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	m	1	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	m	1	NAG	O5-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
3	o	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	l	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	R	2	NAG	C3-C2-N2-C7
3	W	2	NAG	C3-C2-N2-C7

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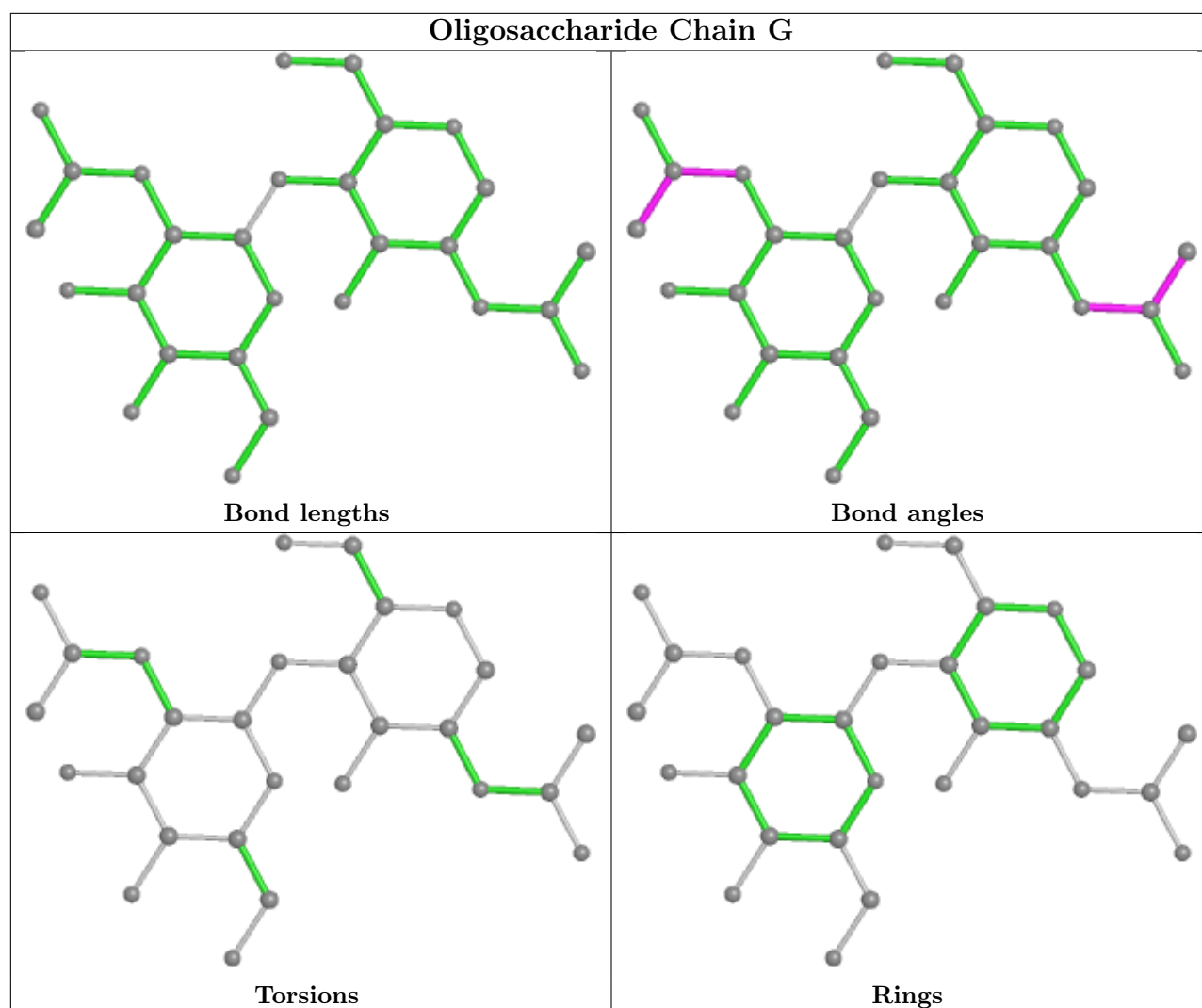
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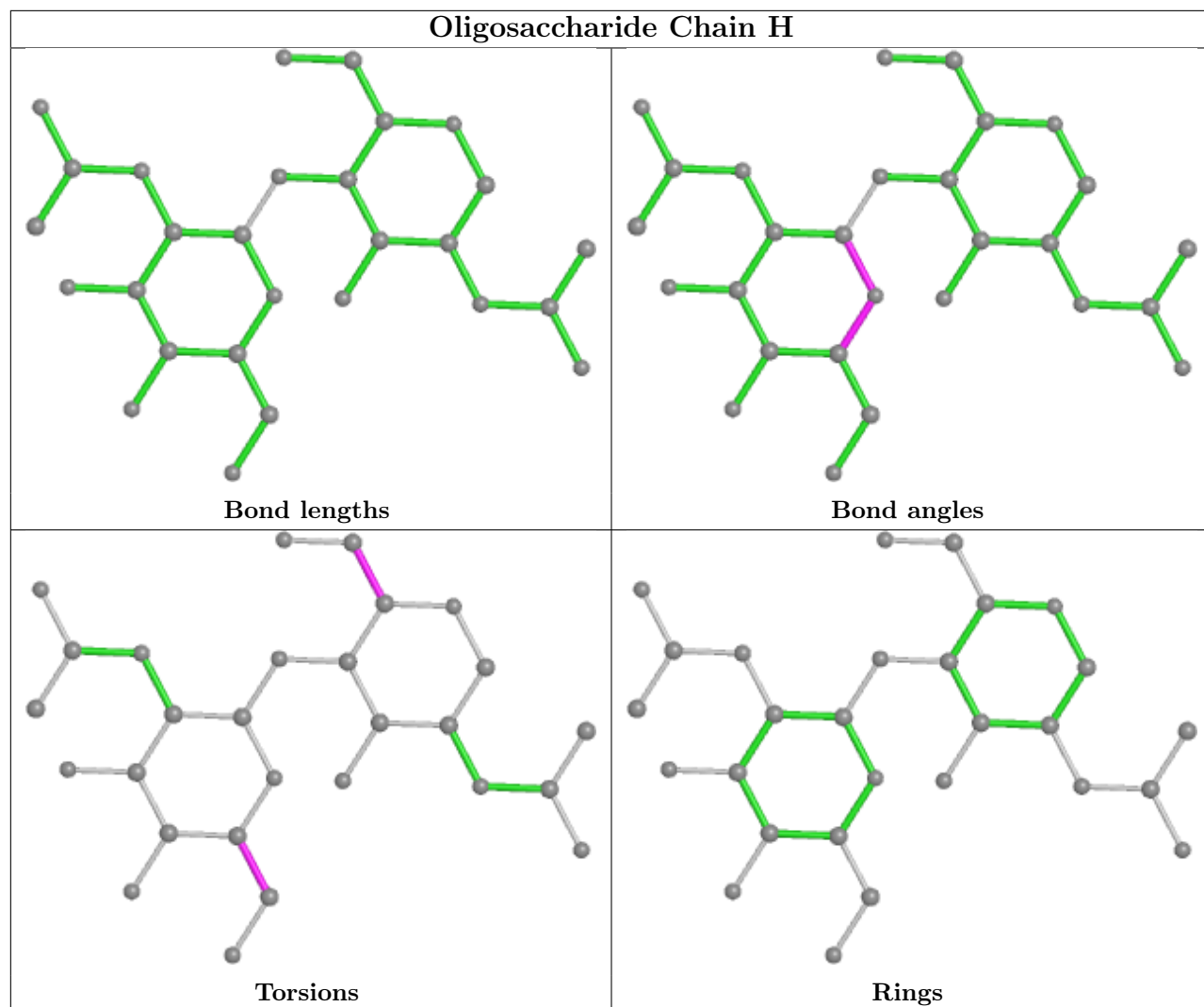
Mol	Chain	Res	Type	Atoms
3	e	1	NAG	C4-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
3	o	1	NAG	C4-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	o	1	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C1-C2-N2-C7
3	Q	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
3	X	2	NAG	C3-C2-N2-C7
3	Y	2	NAG	C3-C2-N2-C7

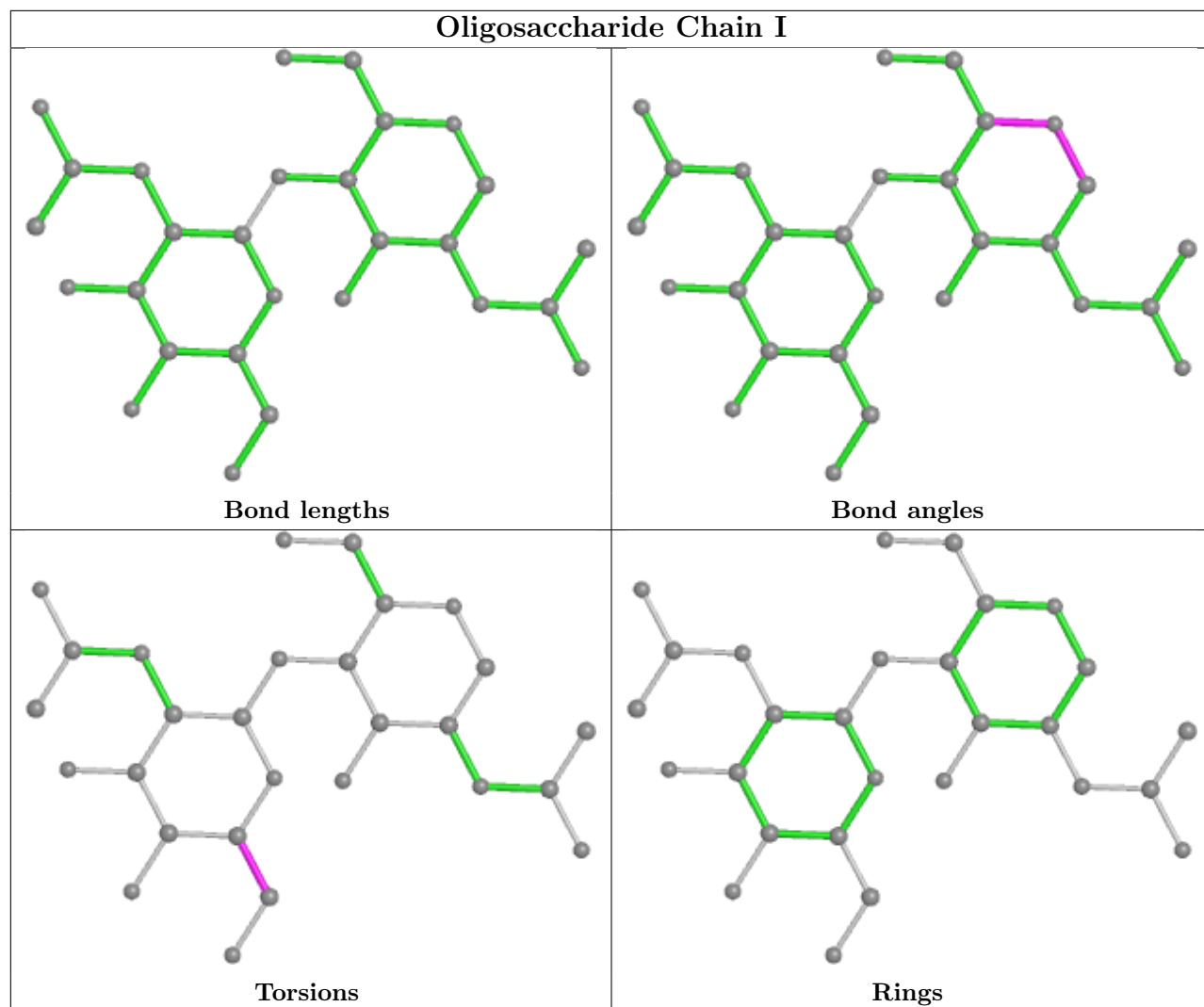
There are no ring outliers.

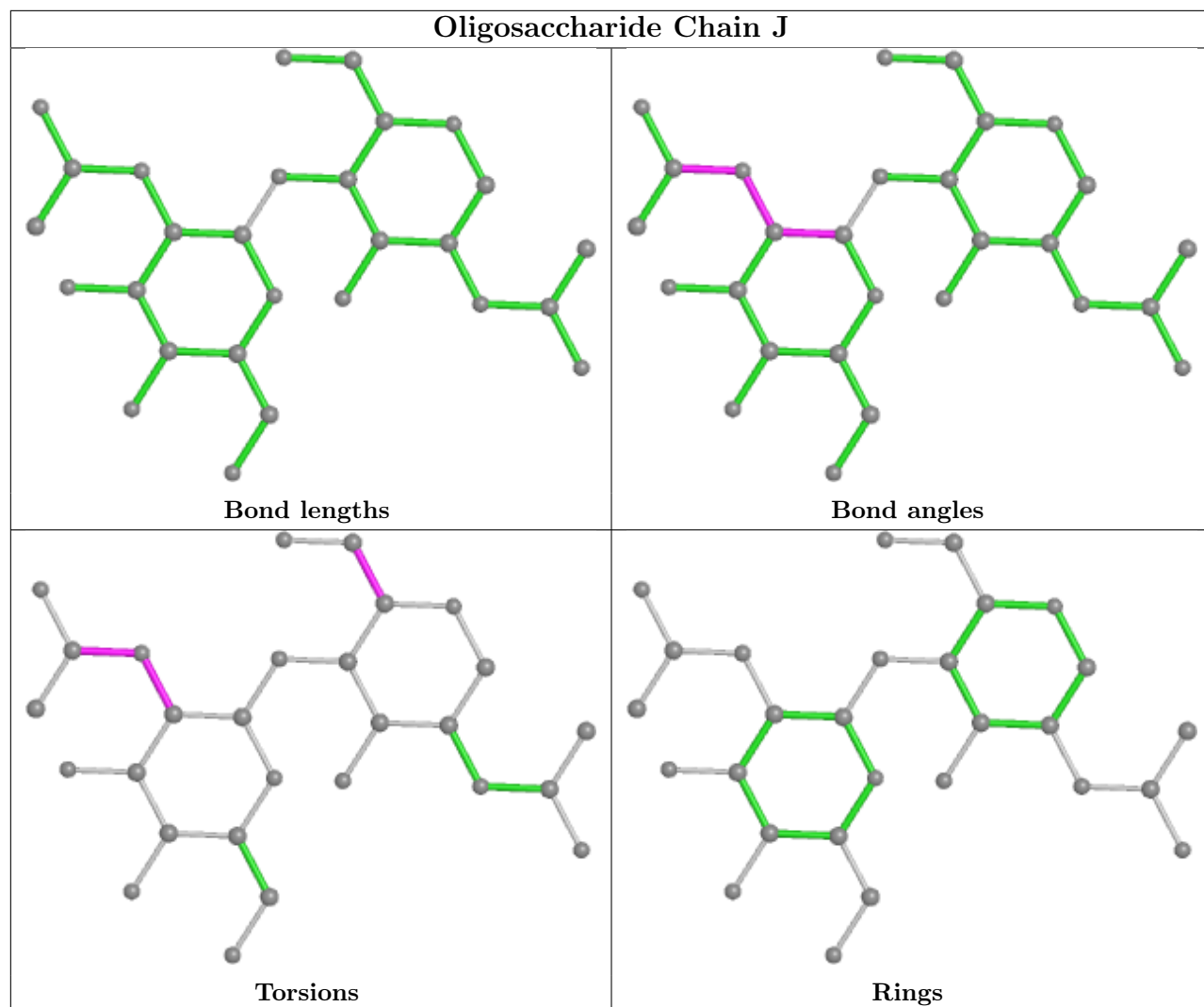
No monomer is involved in short contacts.

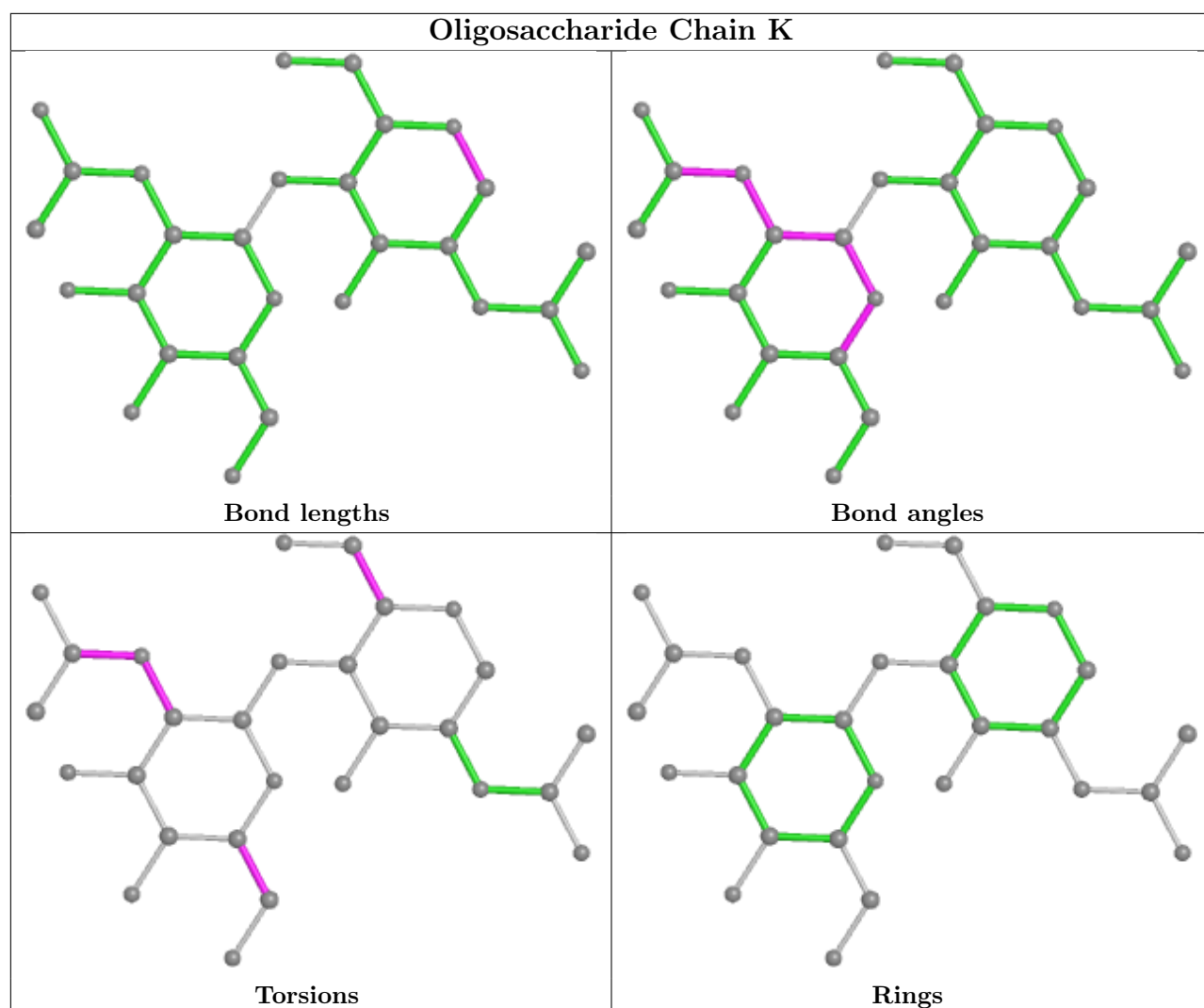
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

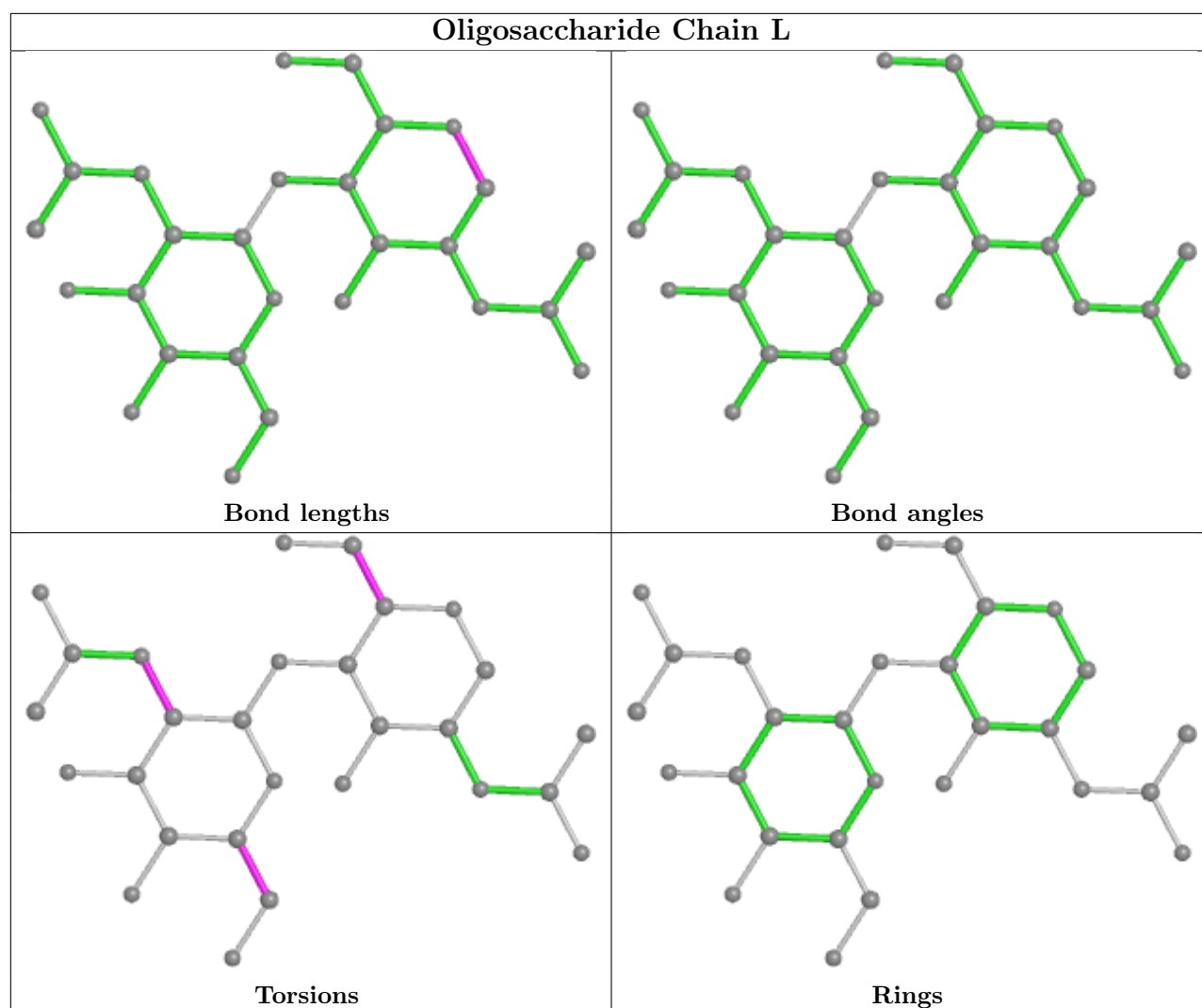


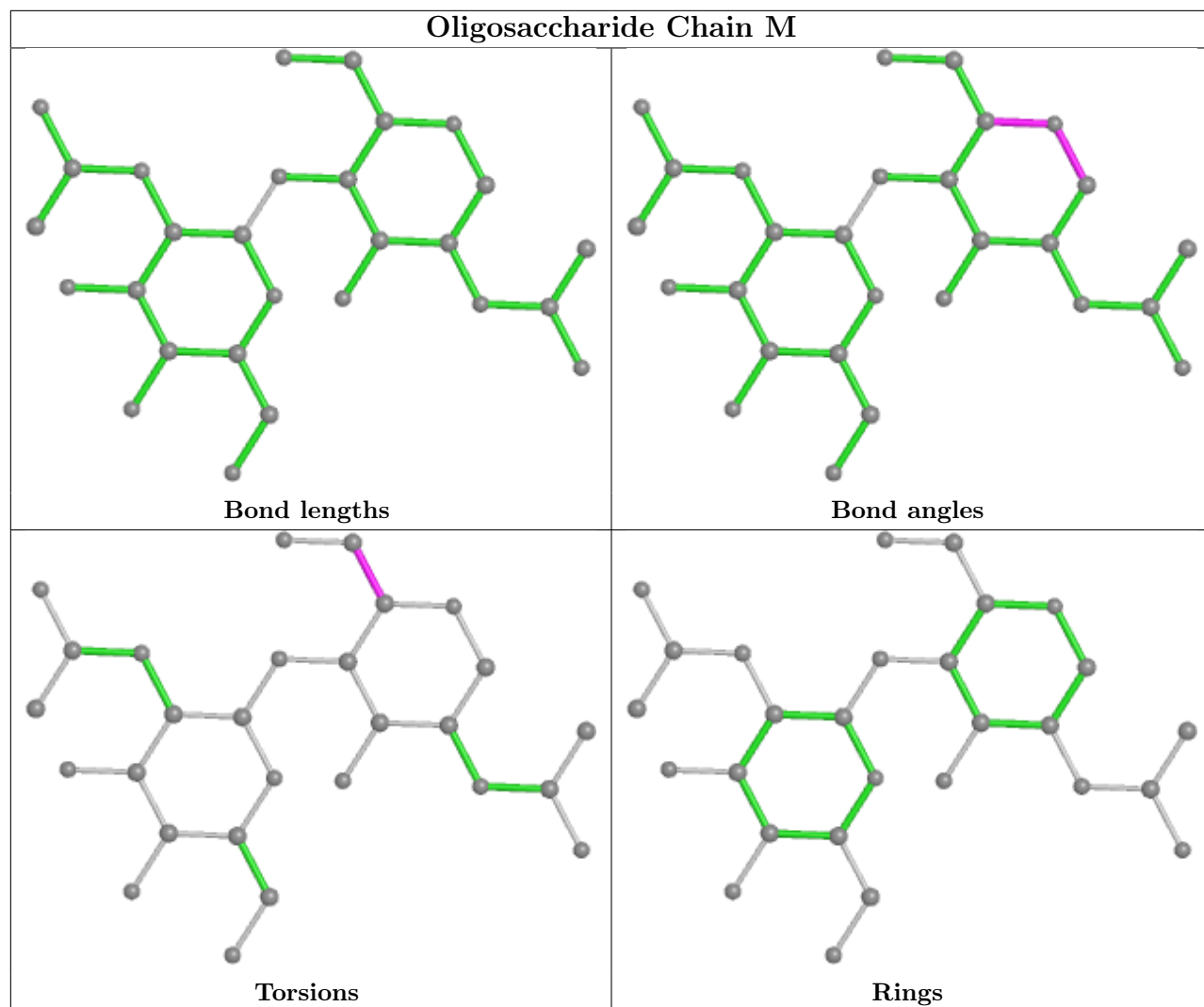


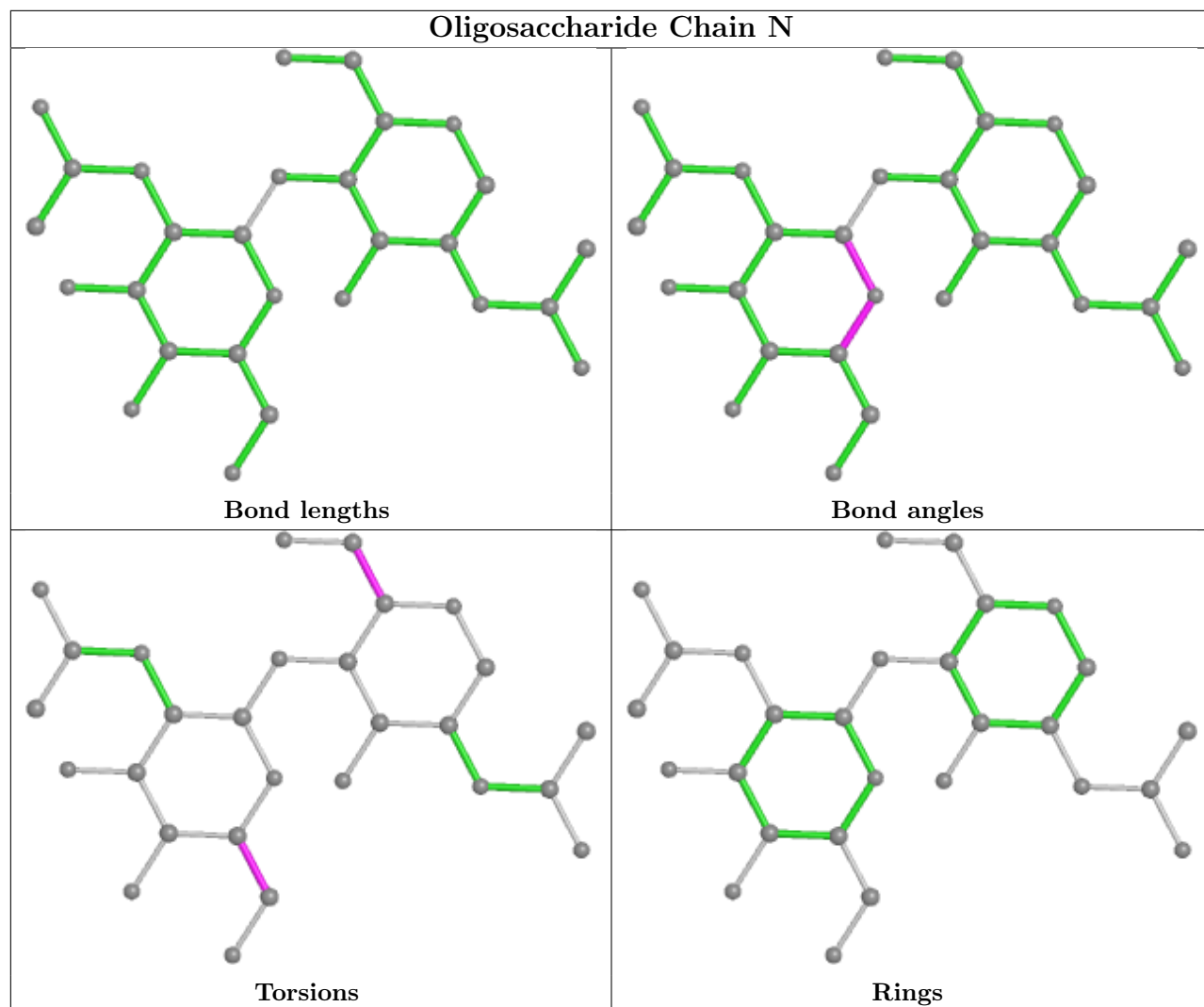


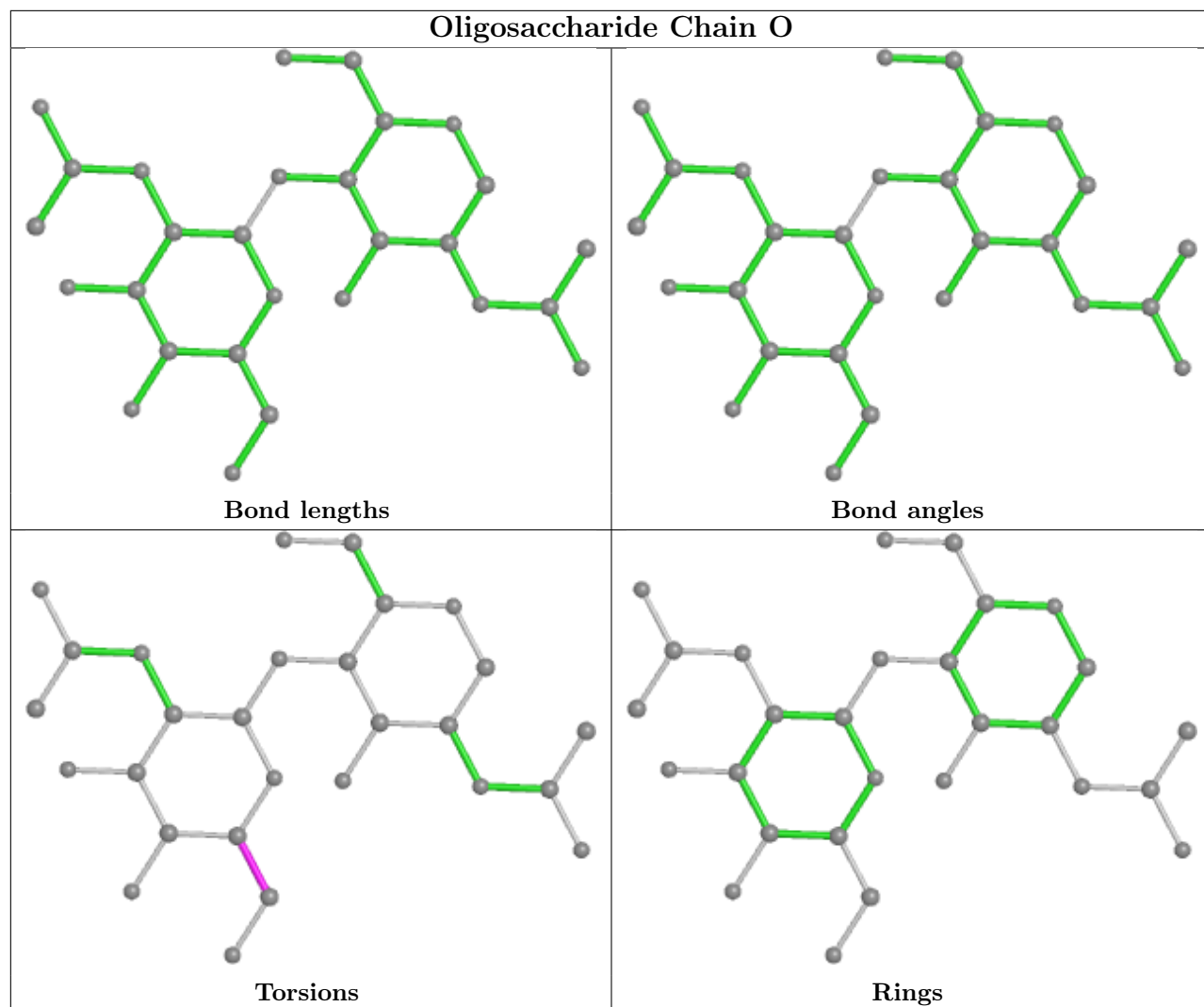


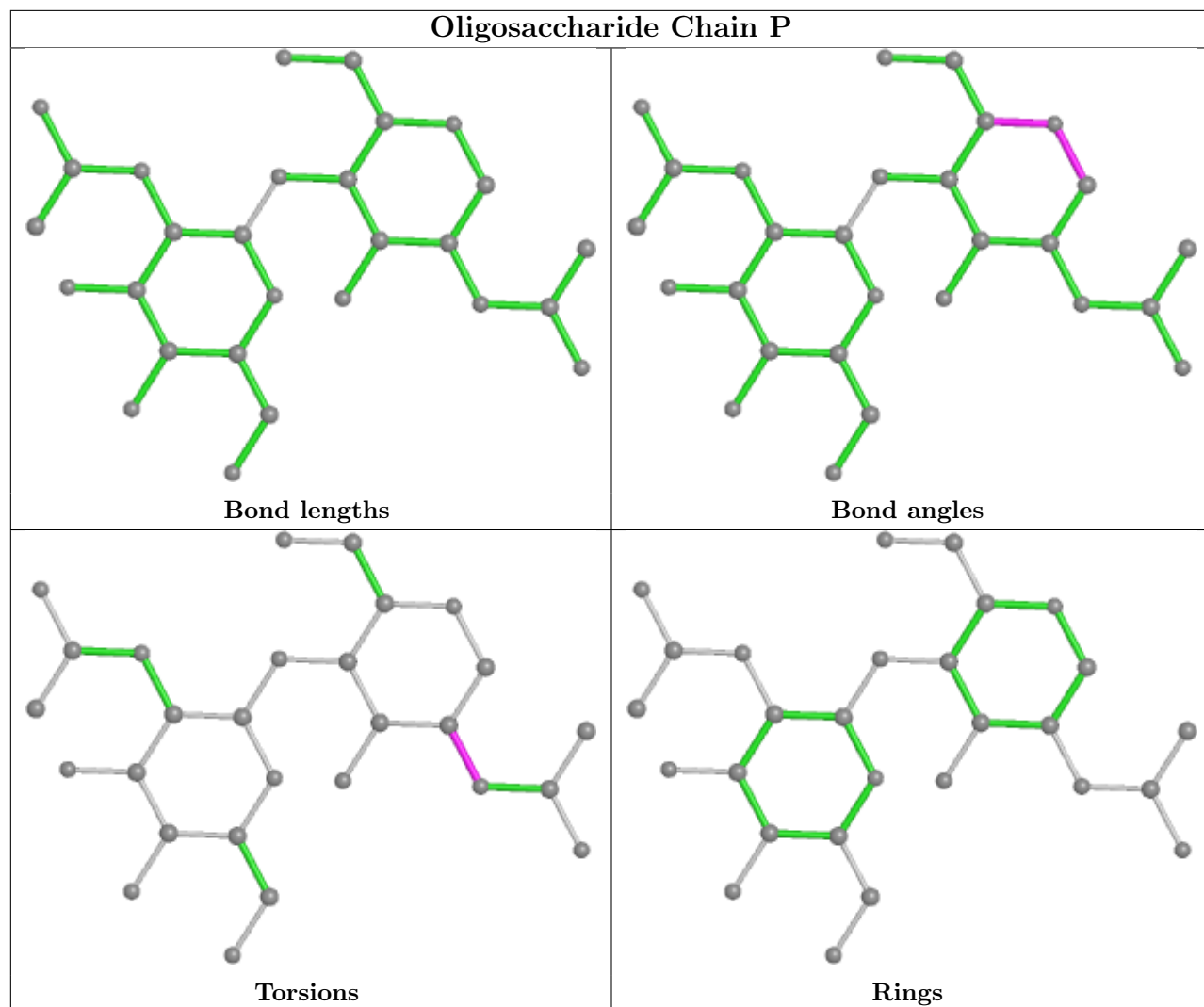


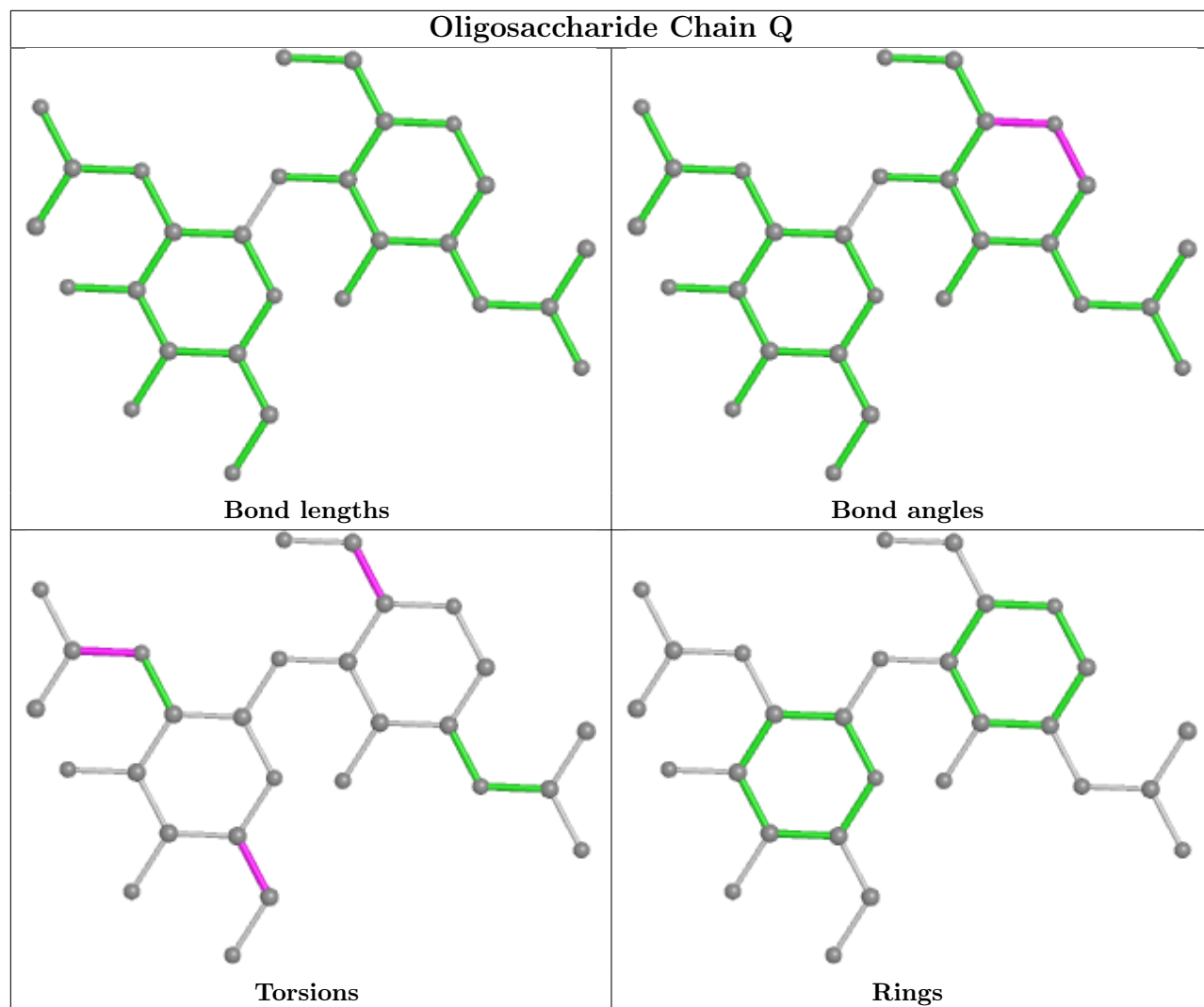


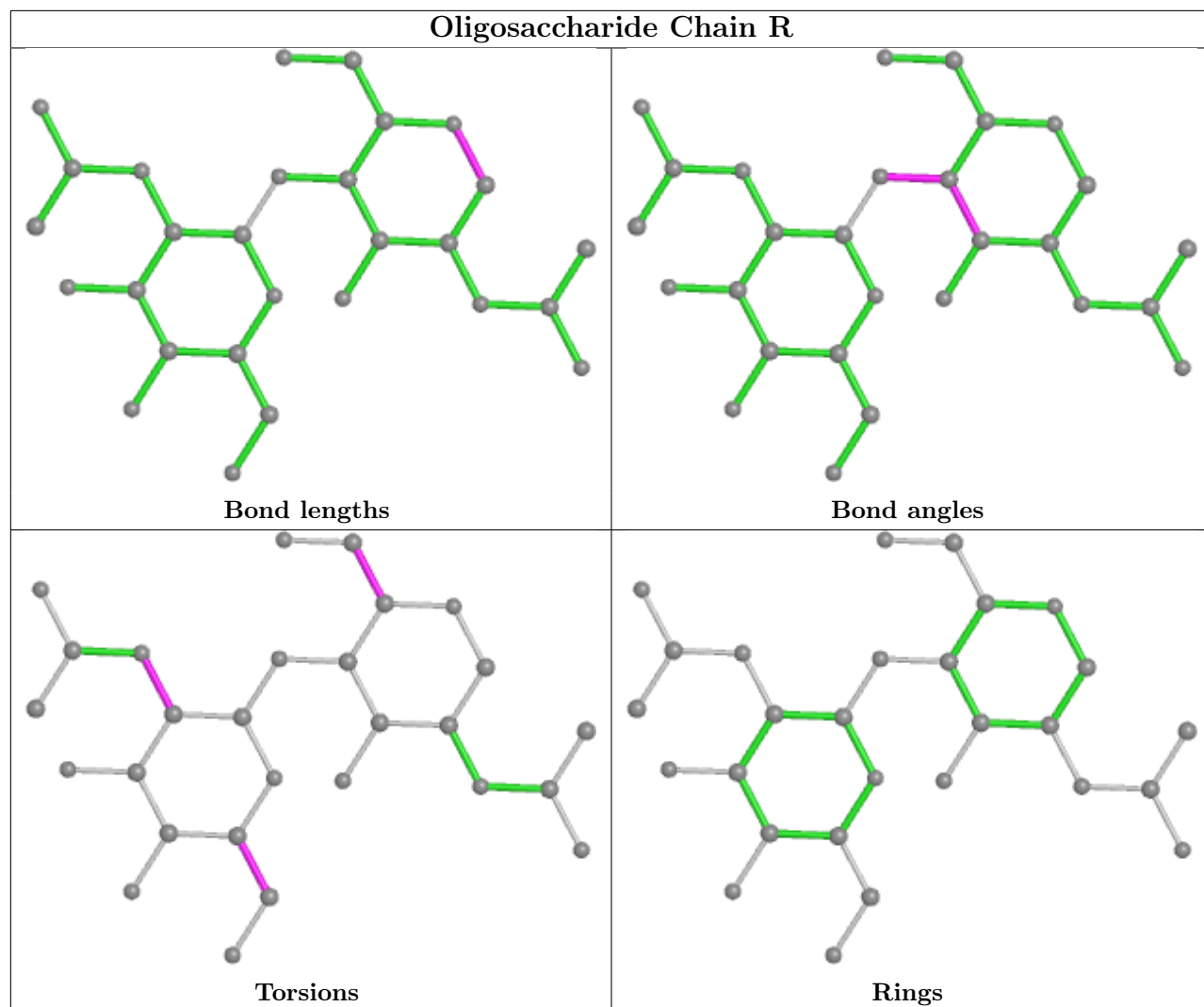


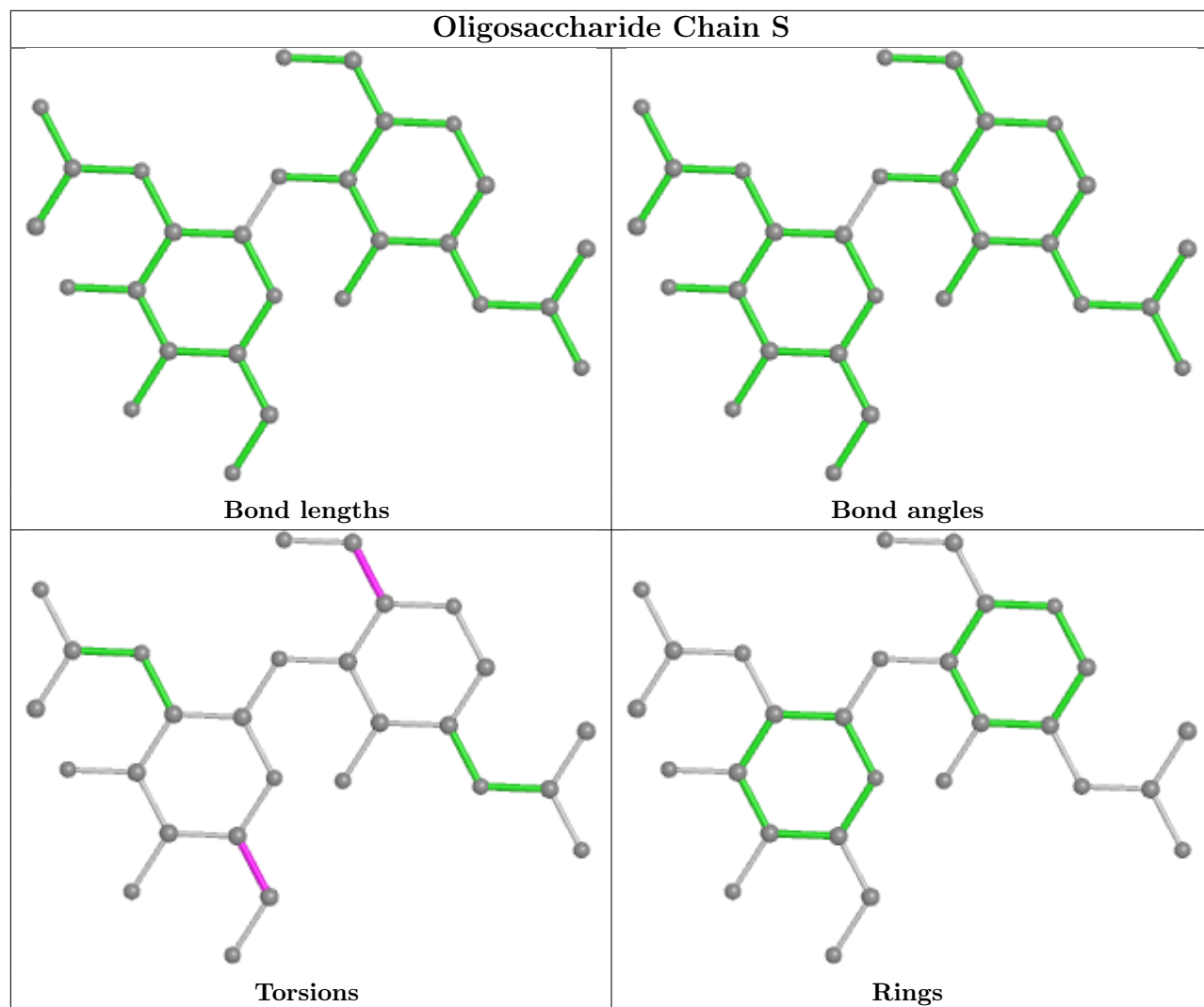


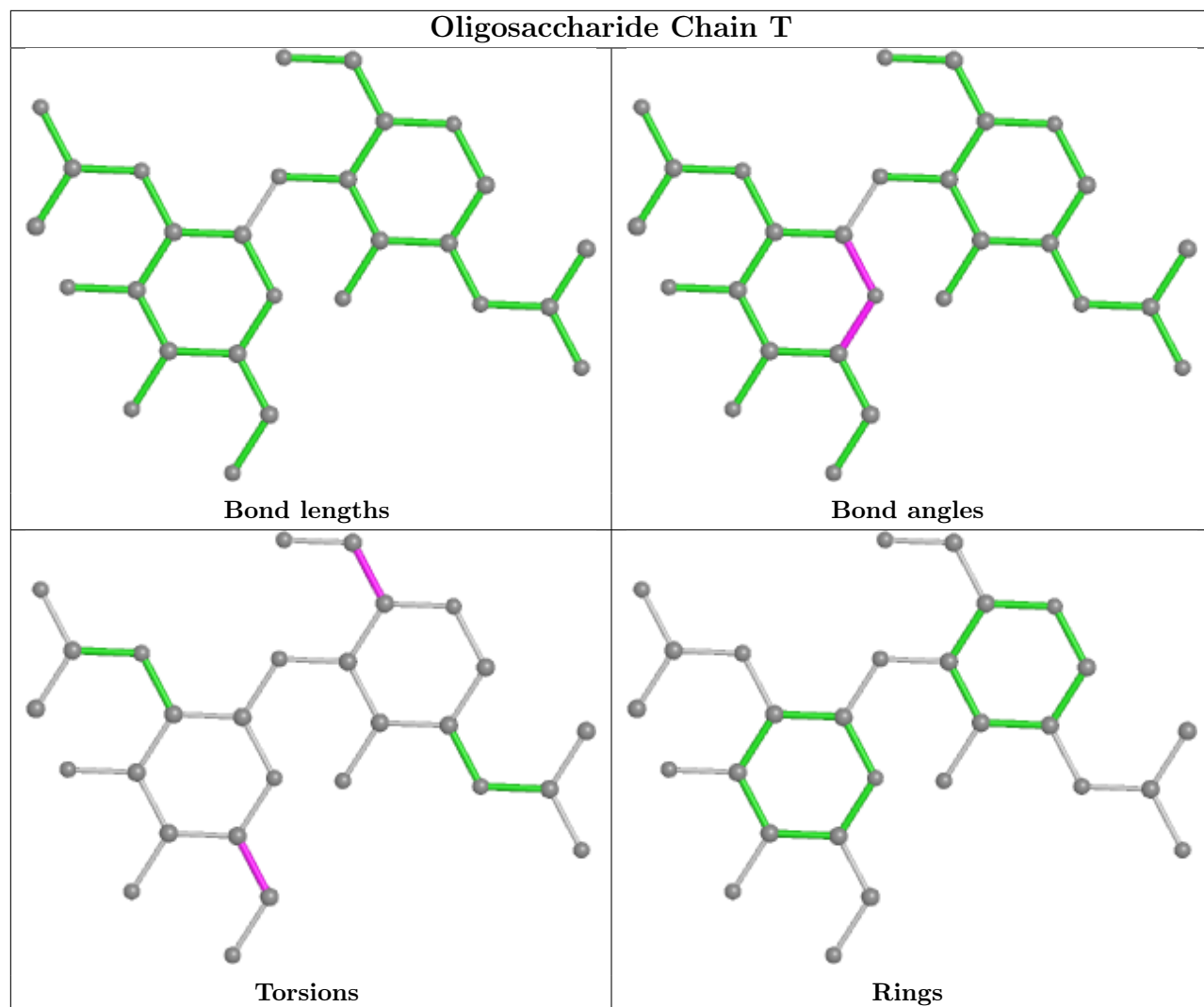


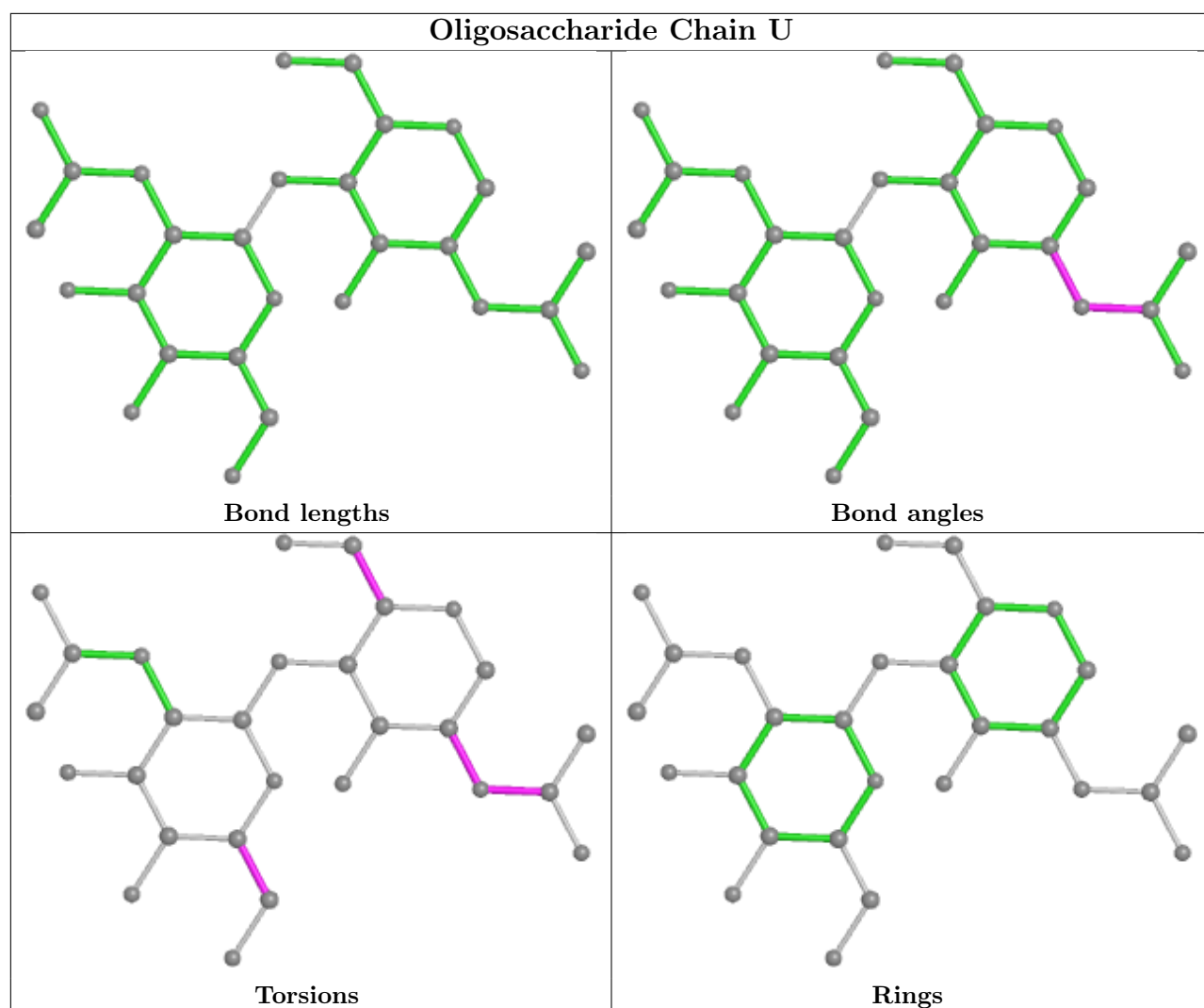


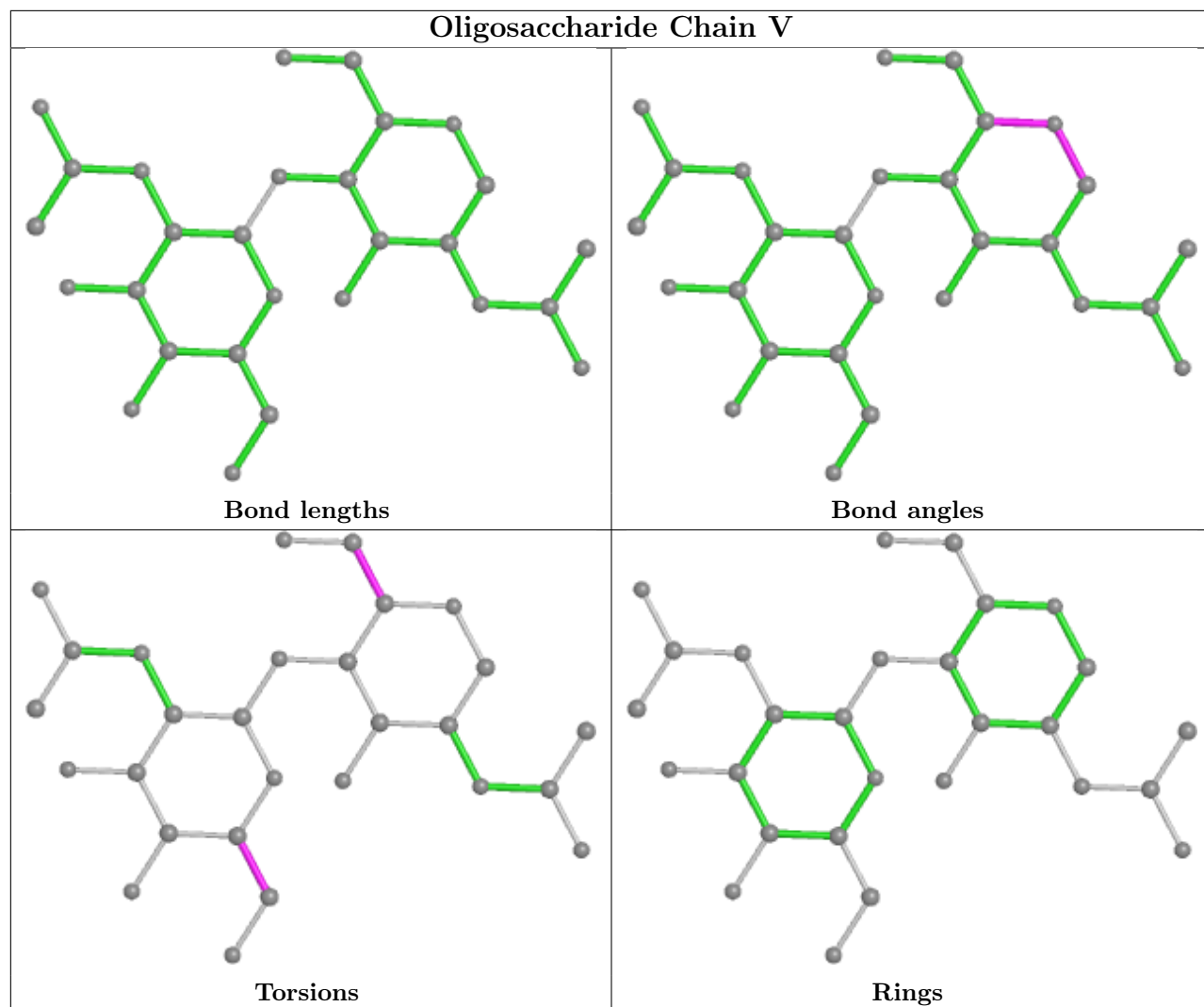


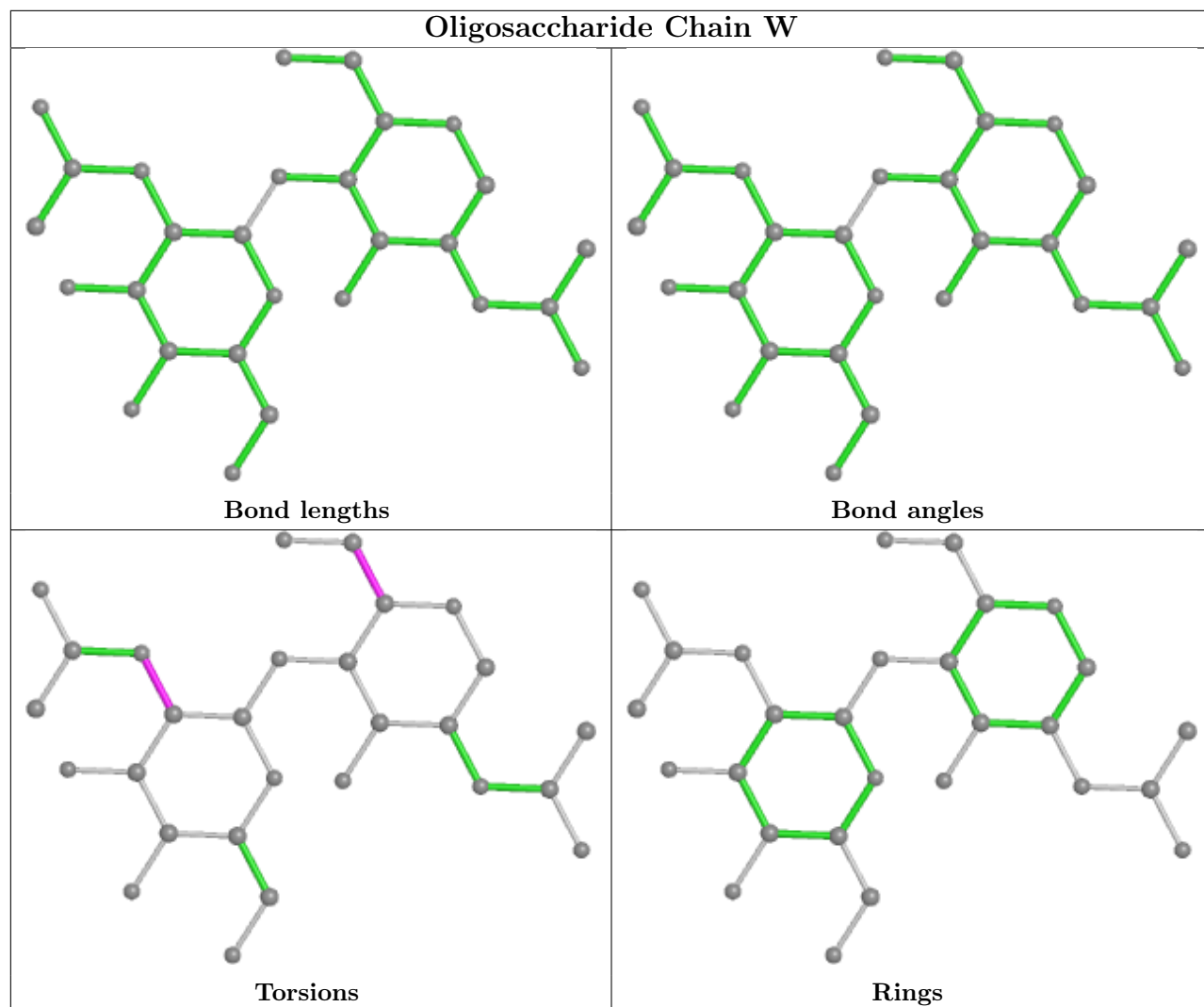


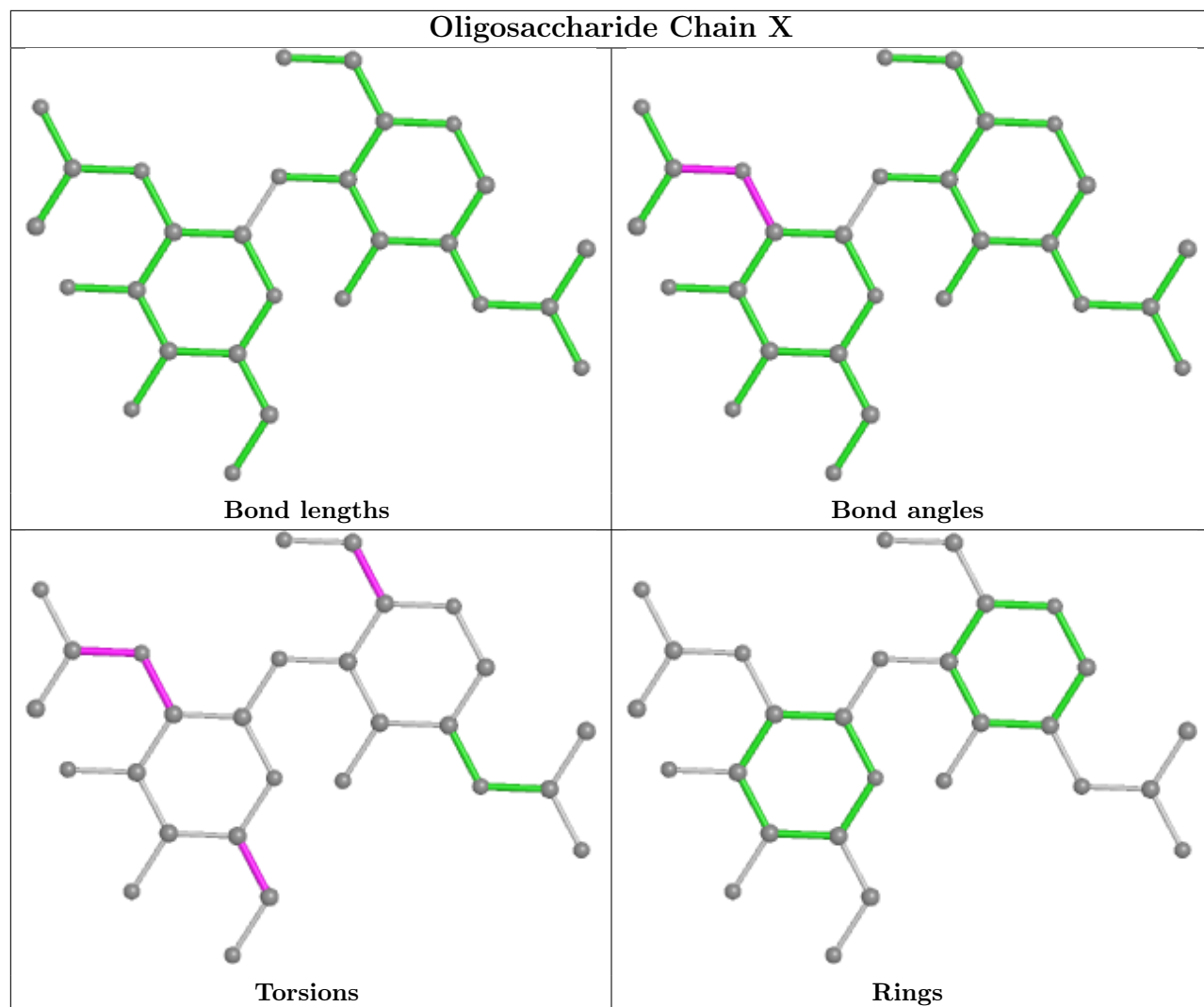


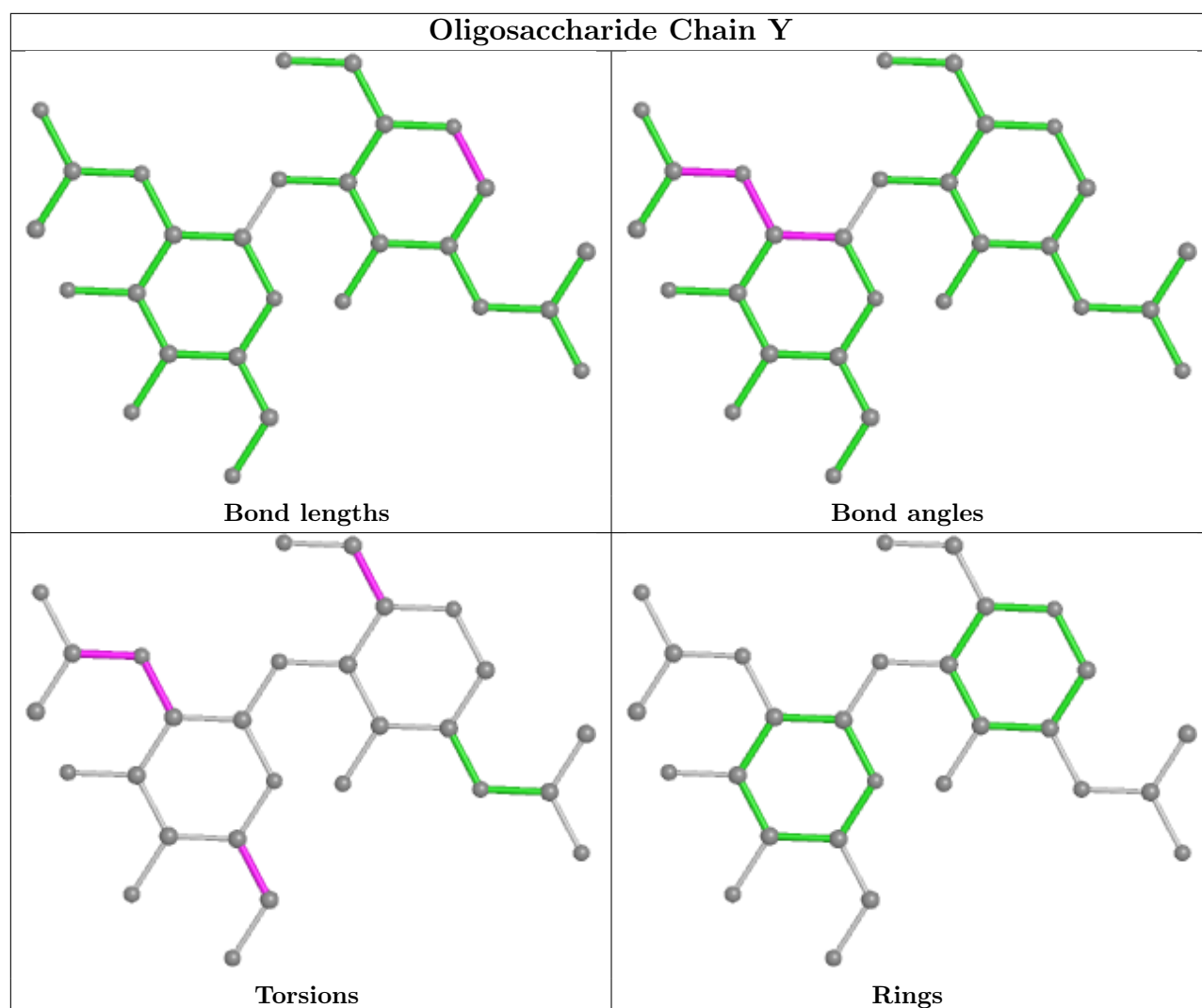


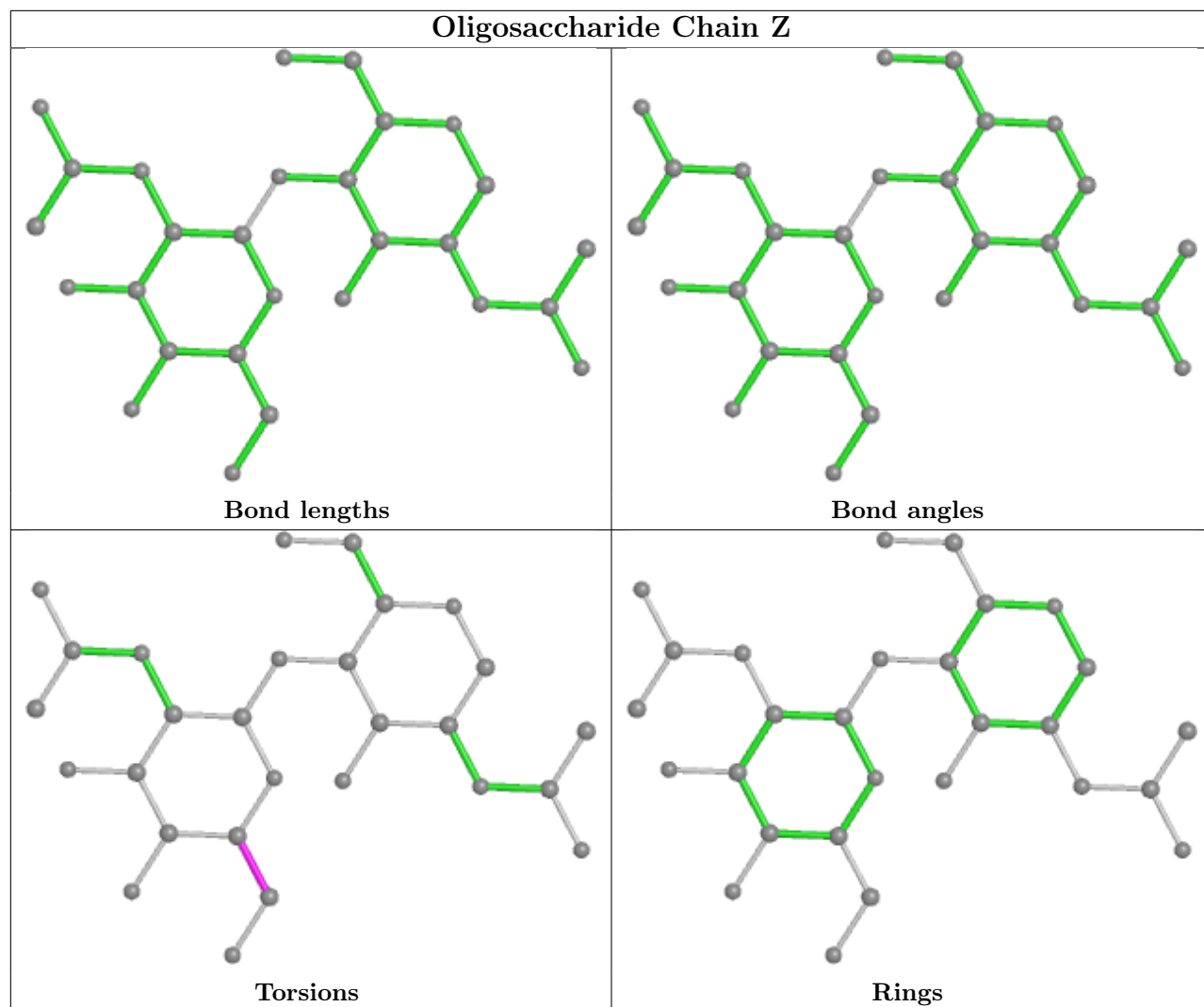


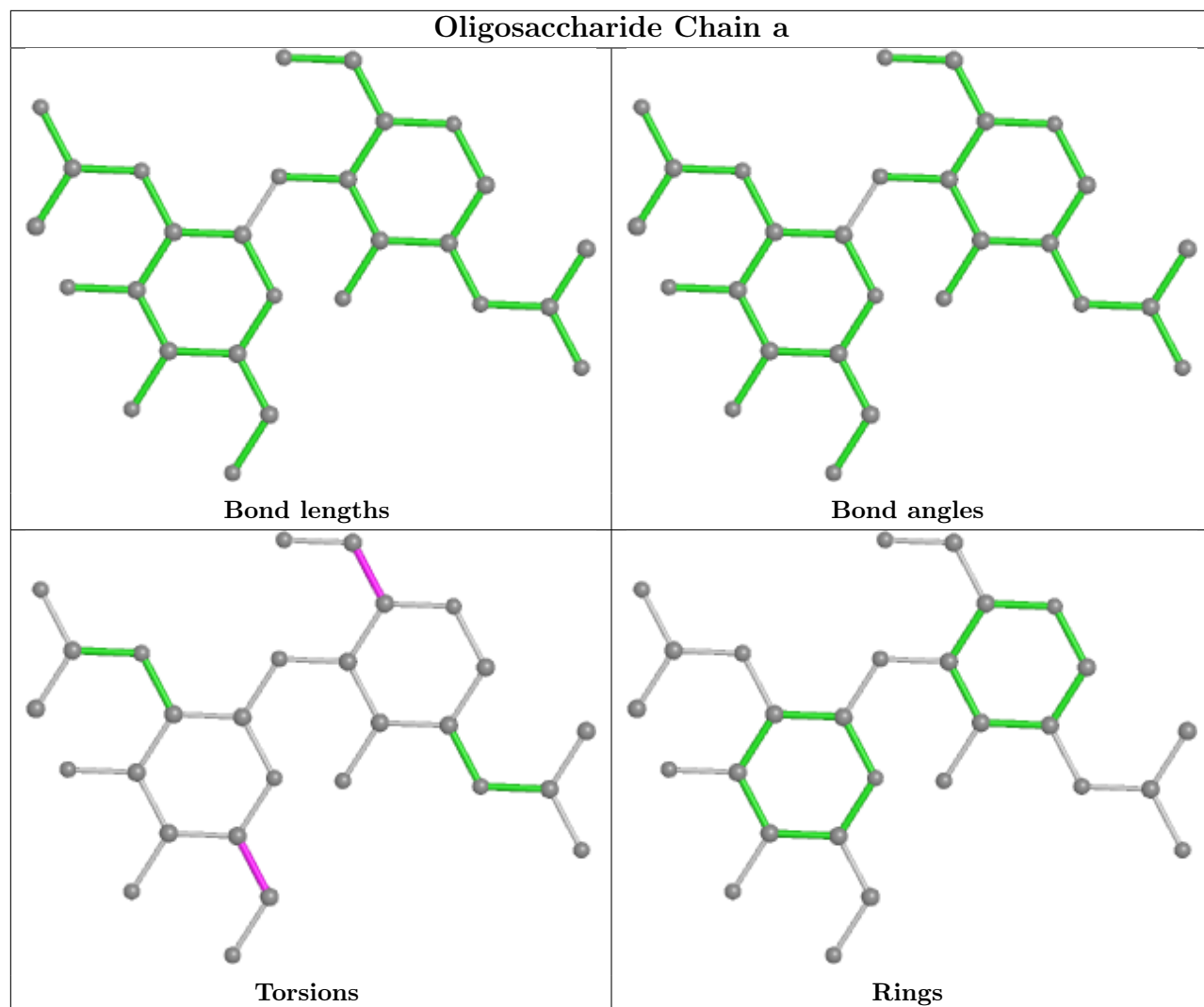


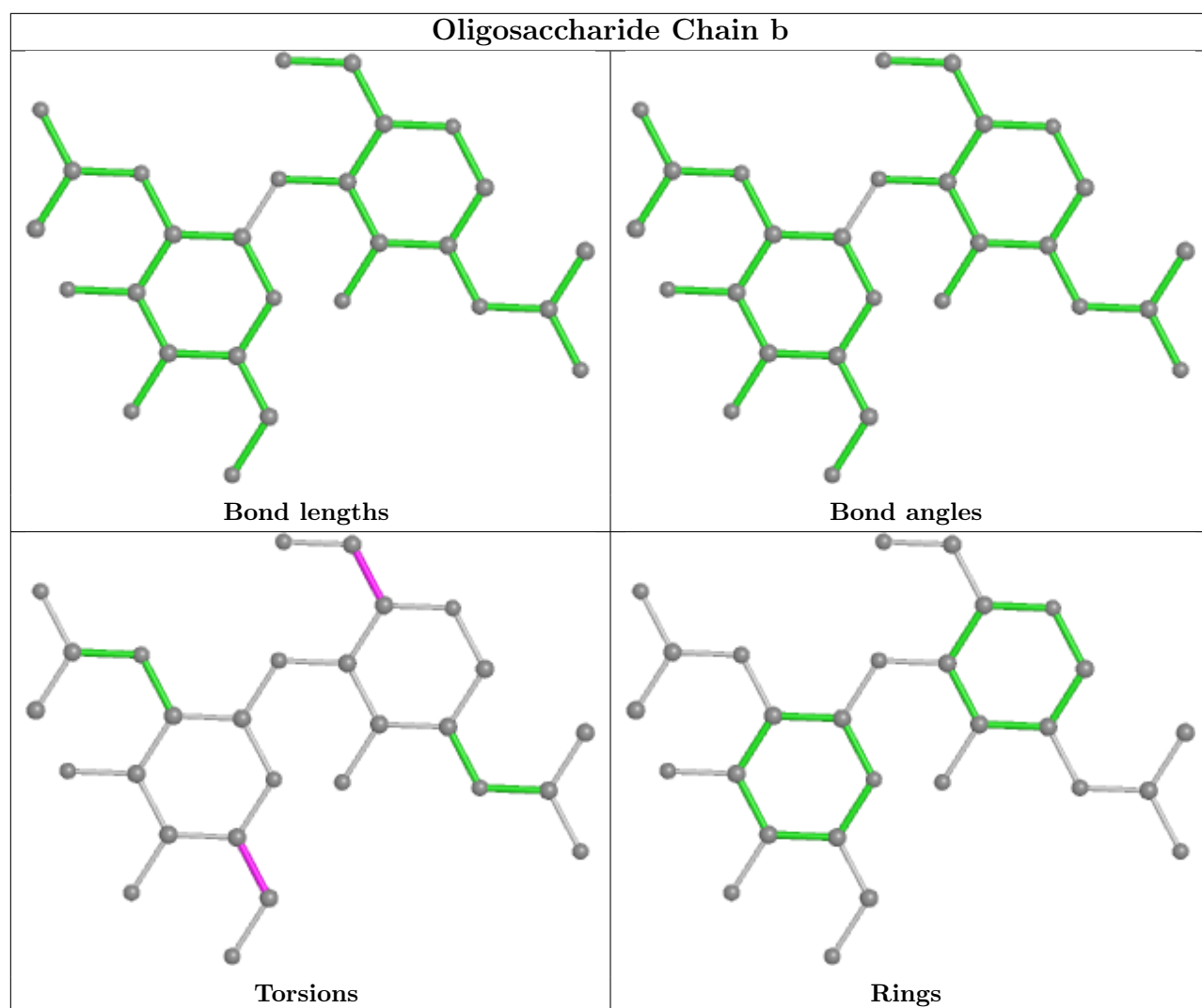


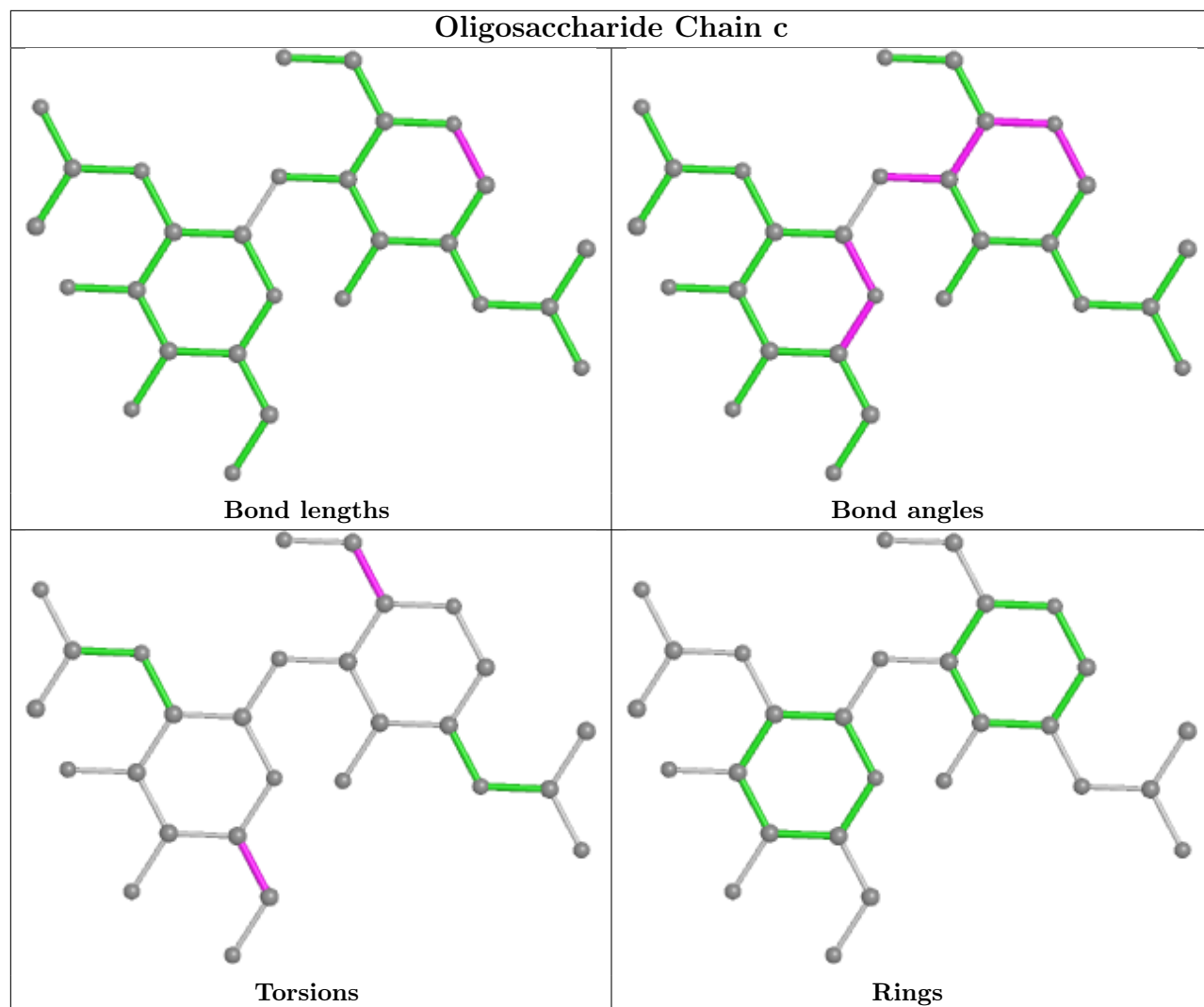


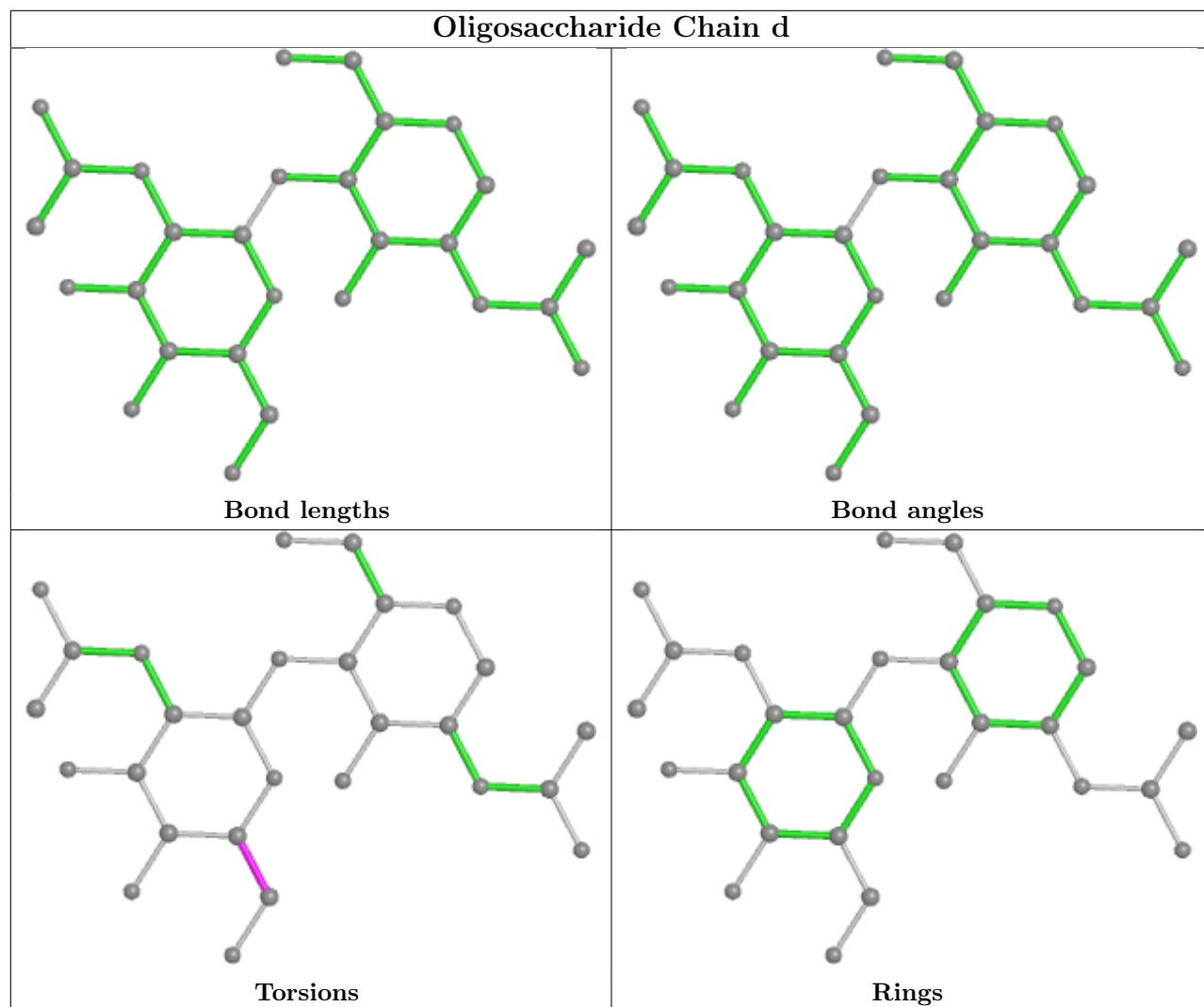


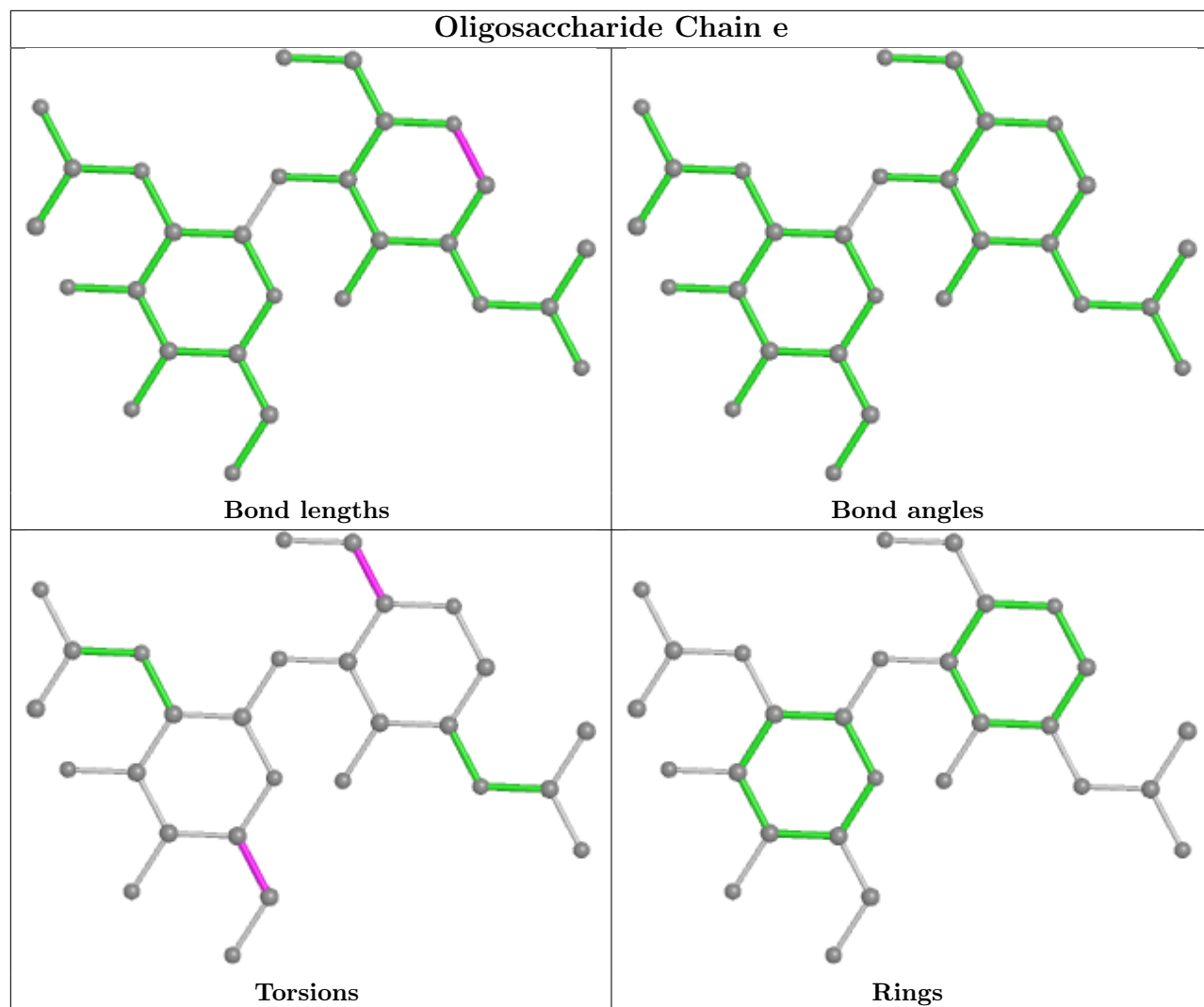


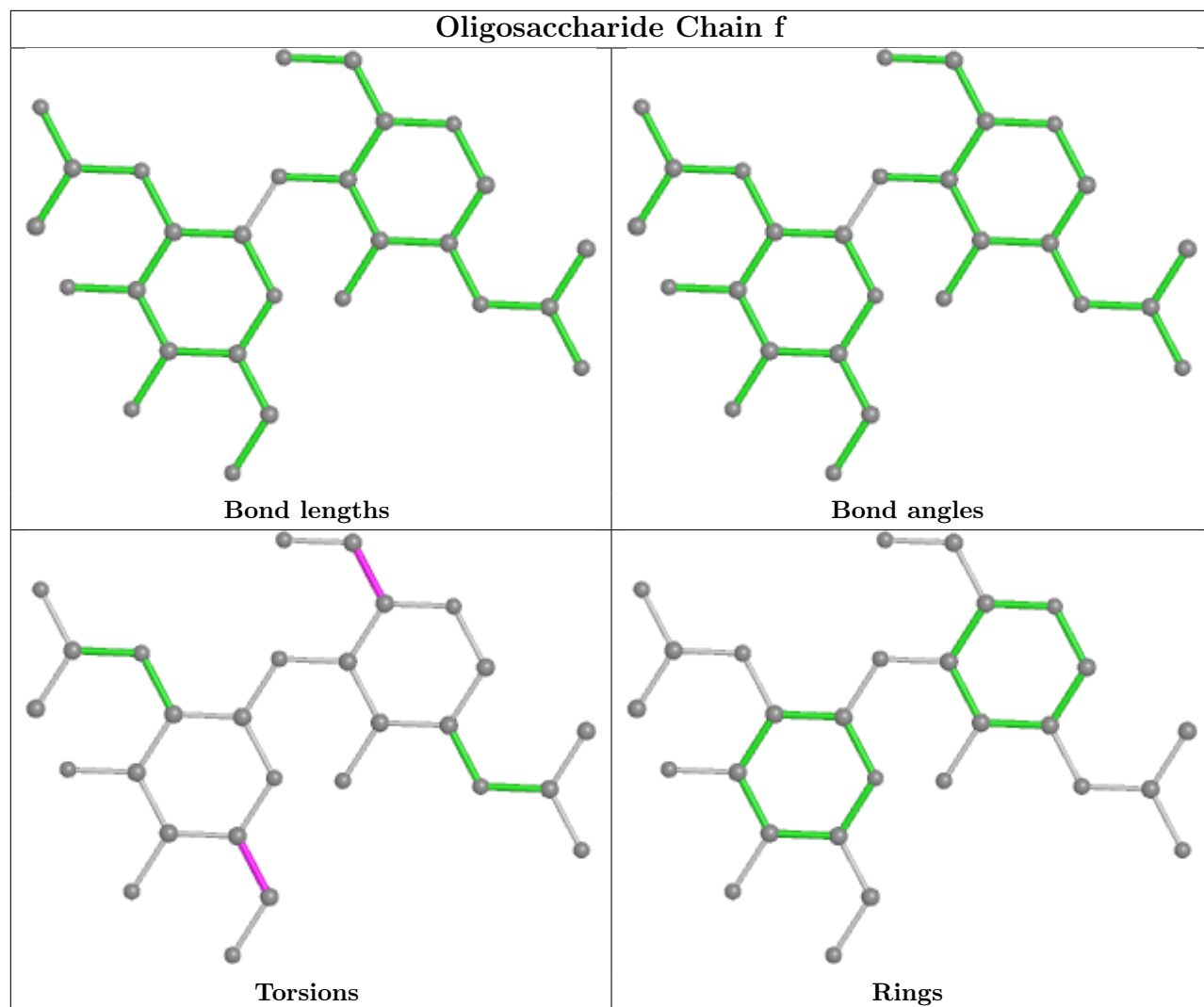


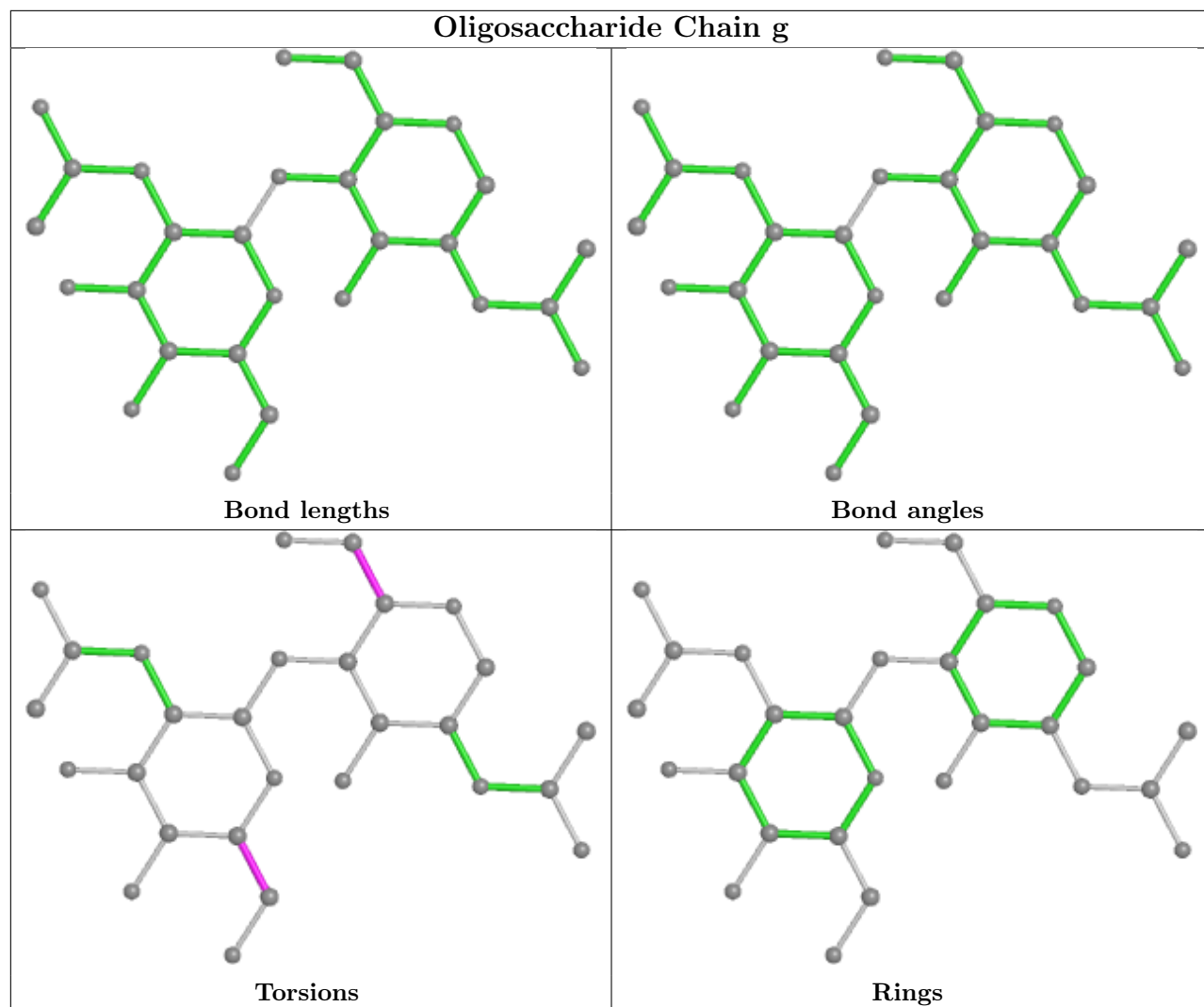


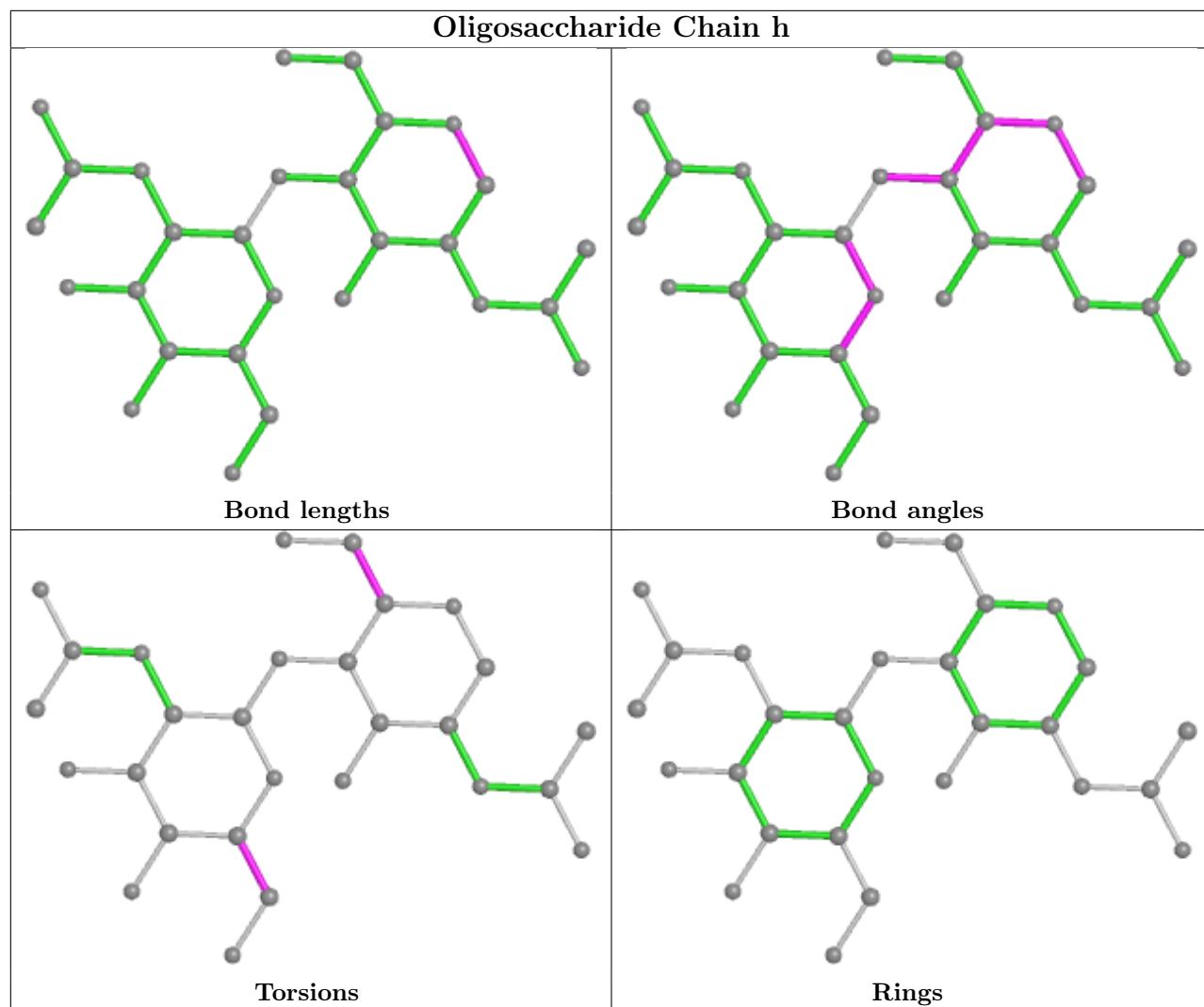


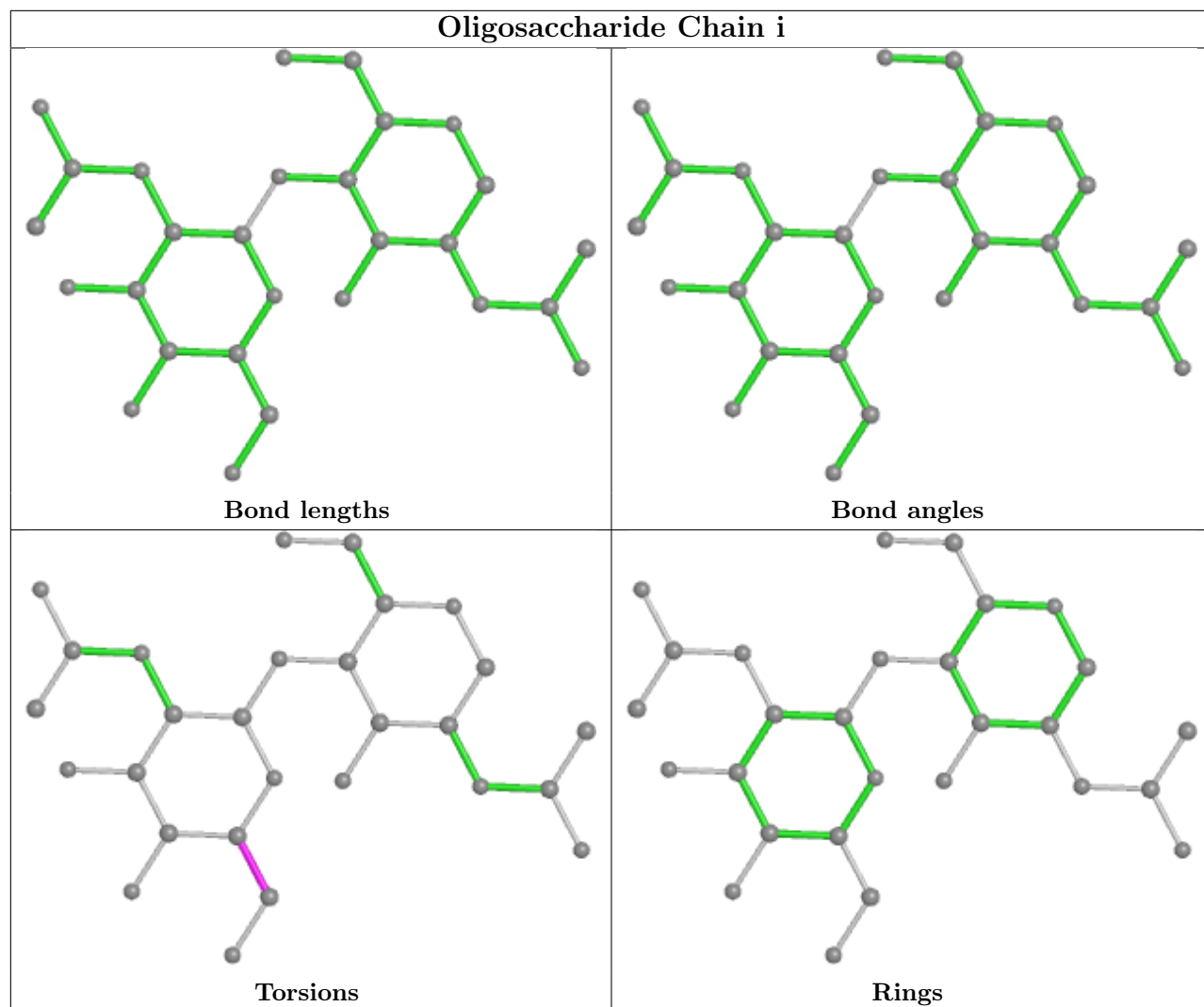


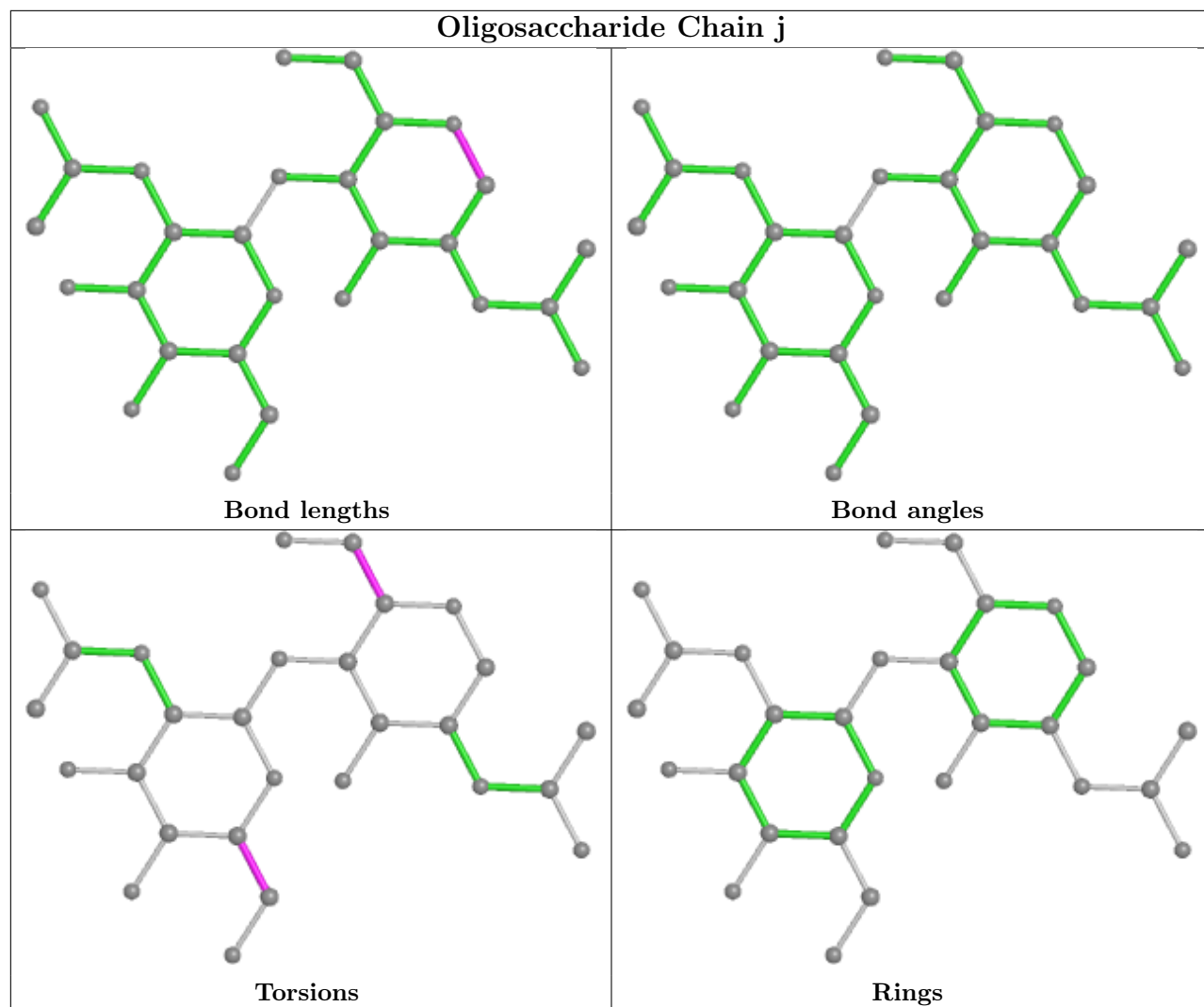


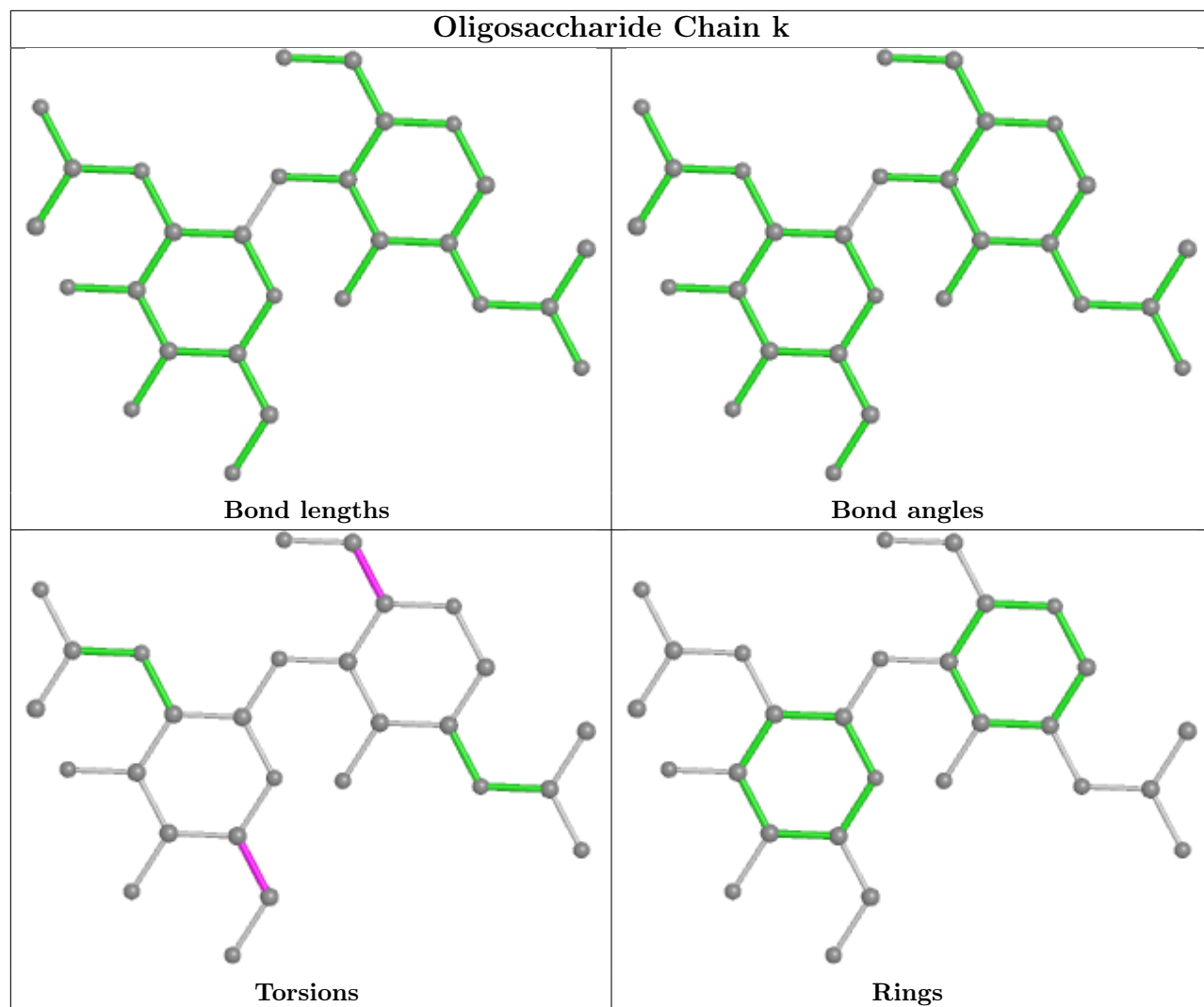


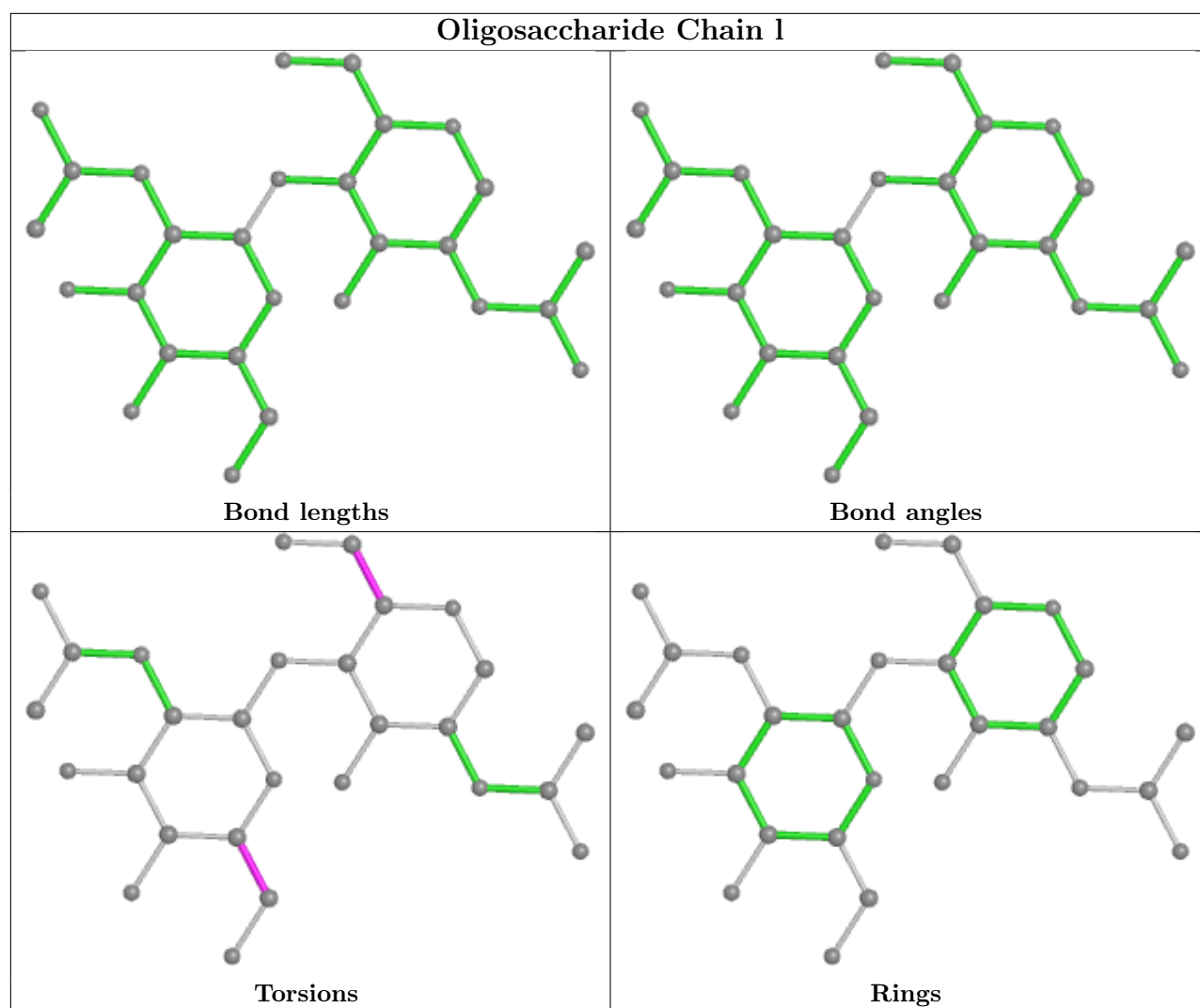


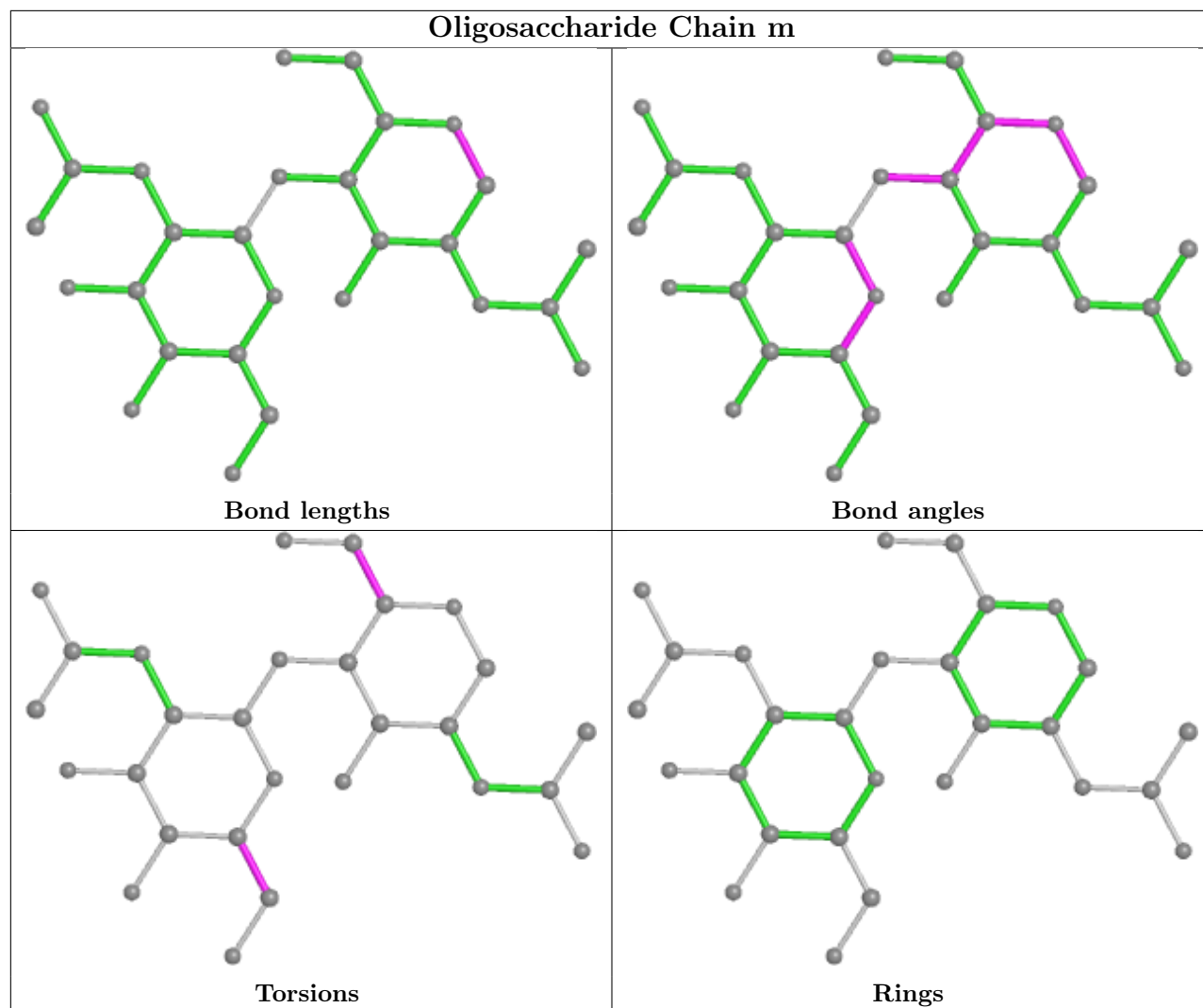


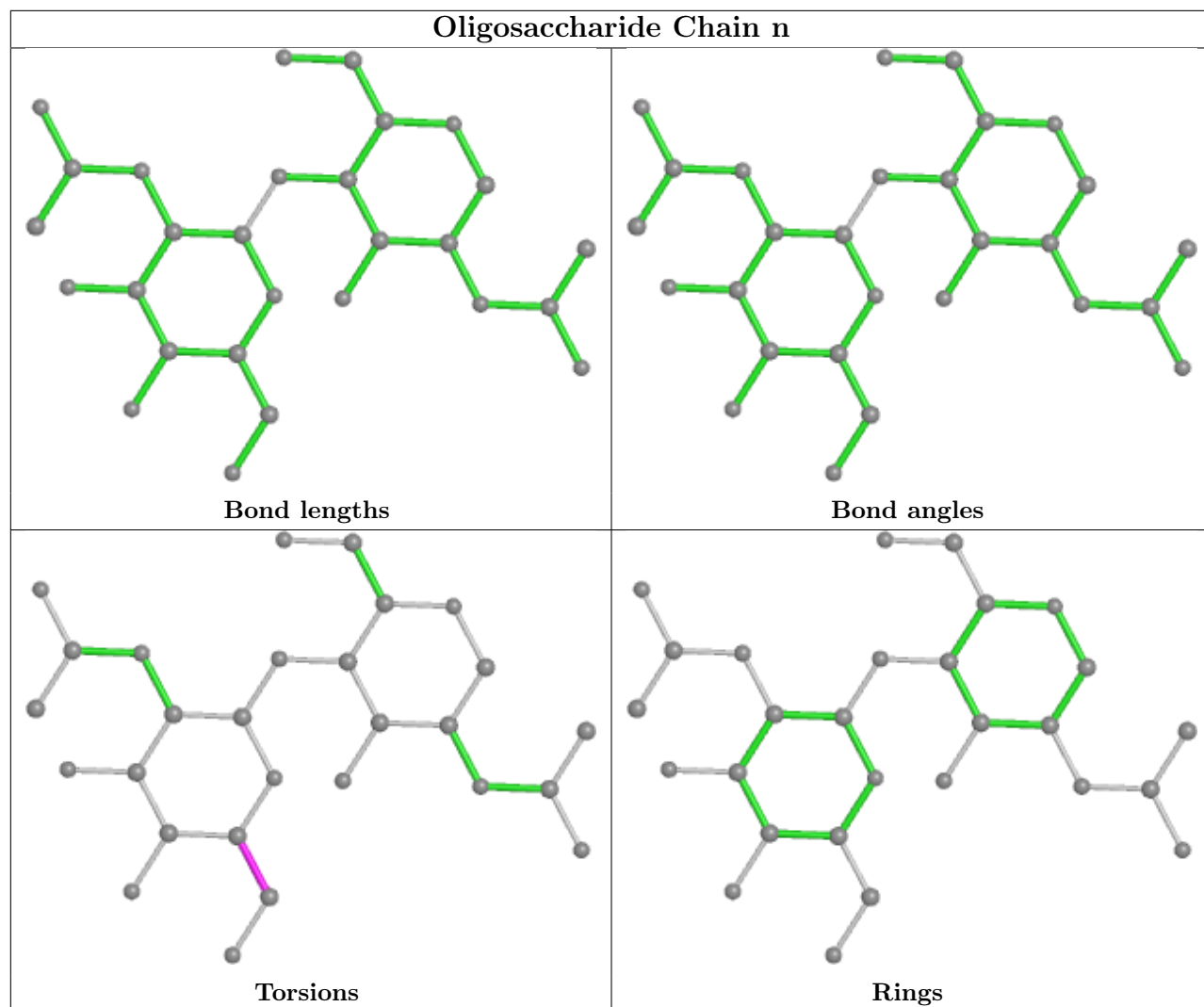


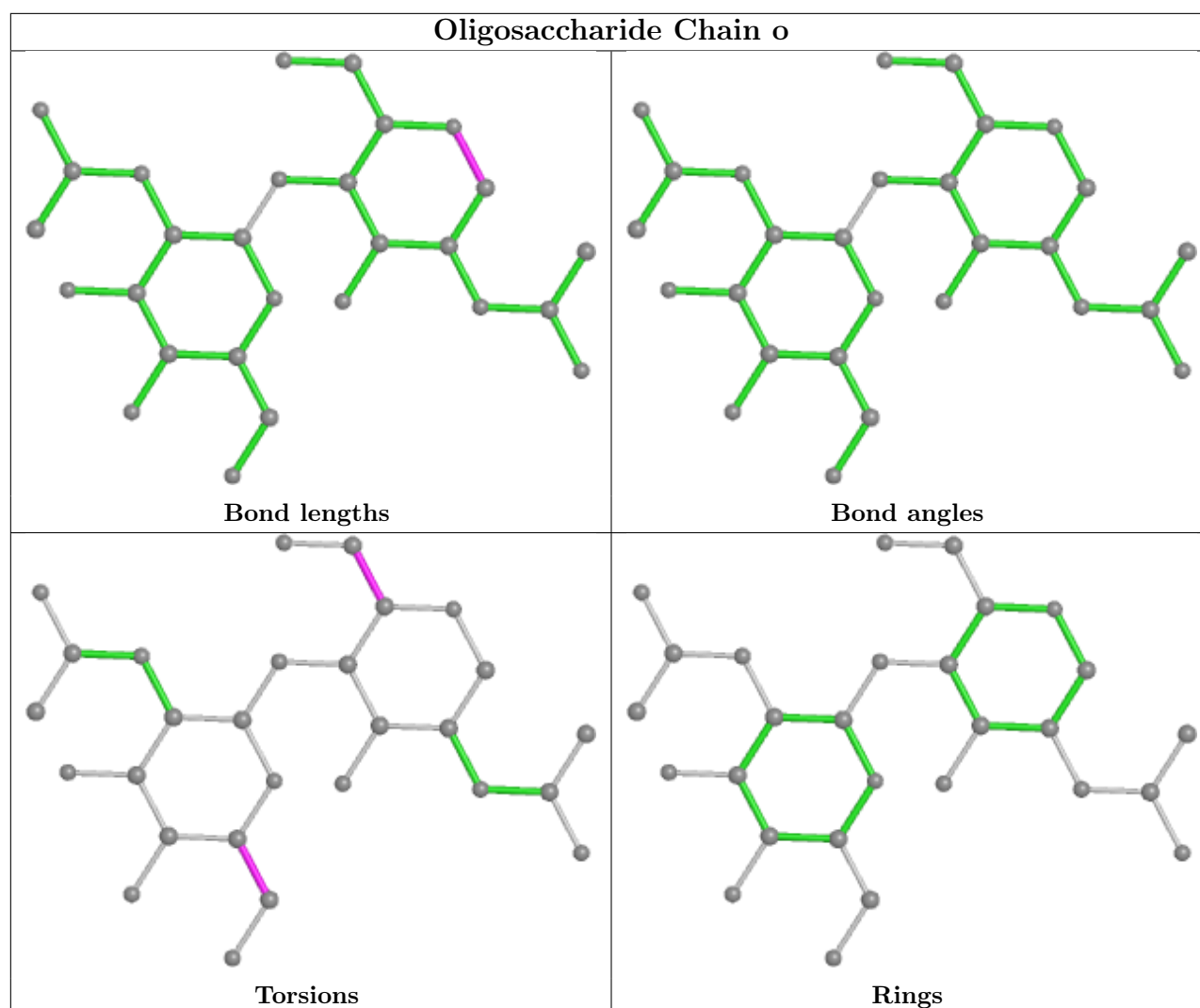












5.6 Ligand geometry [i](#)

34 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1404	1	14,14,15	0.45	0	17,19,21	0.54	0
4	NAG	B	1411	1,4	14,14,15	0.40	0	17,19,21	1.15	1 (5%)
4	NAG	A	1408	1	14,14,15	0.31	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1406	1,4	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
4	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	1407	4	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
4	NAG	B	1406	1,4	14,14,15	0.40	0	17,19,21	1.16	1 (5%)
4	NAG	B	1404	1	14,14,15	0.46	0	17,19,21	0.55	0
4	NAG	C	1404	1	14,14,15	0.46	0	17,19,21	0.54	0
4	NAG	B	1410	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
4	NAG	A	1407	1	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	C	1401	1	14,14,15	0.32	0	17,19,21	0.33	0
4	NAG	B	1403	1	14,14,15	0.19	0	17,19,21	0.39	0
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	C	1403	1	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.62	0
4	NAG	C	1408	1	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	A	1401	1	14,14,15	0.32	0	17,19,21	0.34	0
4	NAG	B	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
4	NAG	B	1401	1	14,14,15	0.32	0	17,19,21	0.33	0
4	NAG	A	1409	1	14,14,15	0.51	0	17,19,21	0.36	0
4	NAG	D	901	2	14,14,15	0.49	0	17,19,21	0.48	0
4	NAG	B	1409	1	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	C	1409	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	C	1410	1	14,14,15	0.31	0	17,19,21	0.38	0
4	NAG	A	1405	1	14,14,15	0.56	0	17,19,21	1.25	1 (5%)
4	NAG	C	1405	1	14,14,15	0.56	0	17,19,21	1.25	1 (5%)
4	NAG	F	901	2	14,14,15	0.49	0	17,19,21	0.47	0
4	NAG	B	1405	1	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
4	NAG	E	901	2	14,14,15	0.49	0	17,19,21	0.48	0
4	NAG	B	1408	1	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
4	NAG	C	1407	4	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
4	NAG	B	1412	4	14,14,15	0.33	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1411	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1407	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	F	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1407	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1412	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1405	NAG	C2-N2-C7	4.27	128.98	122.90
4	A	1405	NAG	C2-N2-C7	4.25	128.96	122.90
4	B	1405	NAG	C2-N2-C7	4.22	128.91	122.90
4	B	1408	NAG	C1-O5-C5	2.41	115.46	112.19
4	C	1406	NAG	C8-C7-N2	2.38	120.13	116.10
4	B	1406	NAG	C8-C7-N2	2.37	120.11	116.10
4	B	1407	NAG	C8-C7-N2	2.35	120.08	116.10
4	C	1407	NAG	C8-C7-N2	2.33	120.05	116.10
4	B	1411	NAG	C8-C7-N2	2.31	120.01	116.10
4	C	1406	NAG	C2-N2-C7	-2.01	120.03	122.90

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	D	901	NAG	O5-C5-C6-O6
4	E	901	NAG	O5-C5-C6-O6
4	F	901	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1402	NAG	C4-C5-C6-O6
4	B	1402	NAG	C4-C5-C6-O6
4	C	1402	NAG	C4-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	A	1405	NAG	O5-C5-C6-O6
4	B	1402	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	C	1402	NAG	O5-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	A	1409	NAG	C4-C5-C6-O6
4	B	1409	NAG	C4-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	C	1410	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	A	1405	NAG	C4-C5-C6-O6
4	B	1405	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1405	NAG	C4-C5-C6-O6
4	A	1405	NAG	C8-C7-N2-C2
4	A	1405	NAG	O7-C7-N2-C2
4	B	1405	NAG	C8-C7-N2-C2
4	B	1405	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	A	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
4	C	1408	NAG	C4-C5-C6-O6
4	B	1408	NAG	C4-C5-C6-O6
4	D	901	NAG	C4-C5-C6-O6
4	E	901	NAG	C4-C5-C6-O6
4	F	901	NAG	C4-C5-C6-O6
4	A	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	C	1403	NAG	O5-C5-C6-O6
4	A	1403	NAG	O5-C5-C6-O6
4	B	1403	NAG	O5-C5-C6-O6
4	A	1403	NAG	C4-C5-C6-O6
4	B	1403	NAG	C4-C5-C6-O6
4	C	1403	NAG	C4-C5-C6-O6
4	B	1410	NAG	C4-C5-C6-O6
4	A	1408	NAG	C4-C5-C6-O6
4	C	1410	NAG	C4-C5-C6-O6
4	B	1410	NAG	O5-C5-C6-O6
4	A	1401	NAG	C4-C5-C6-O6
4	B	1401	NAG	C4-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
4	A	1407	NAG	C1-C2-N2-C7
4	B	1408	NAG	C3-C2-N2-C7
4	C	1409	NAG	C1-C2-N2-C7
4	A	1405	NAG	C3-C2-N2-C7
4	B	1405	NAG	C3-C2-N2-C7
4	C	1405	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

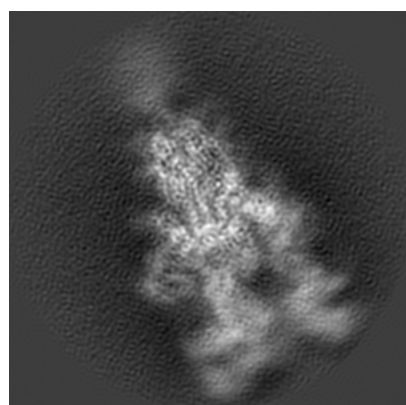
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30460. These allow visual inspection of the internal detail of the map and identification of artifacts.

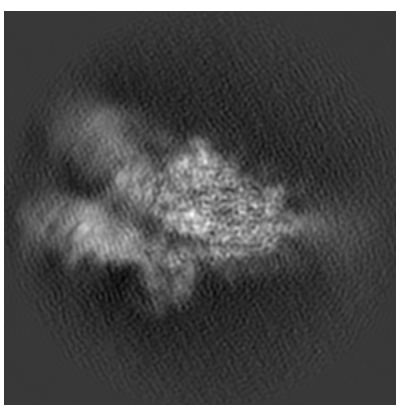
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

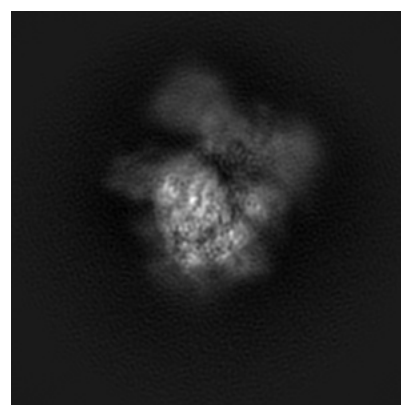
6.1.1 Primary map



X



Y

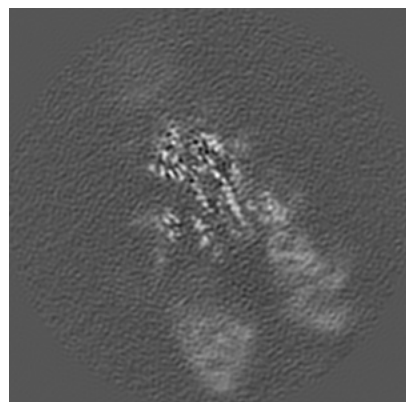


Z

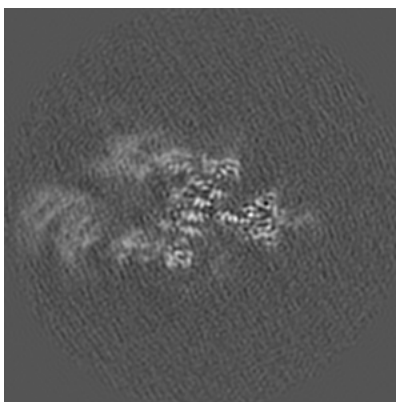
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

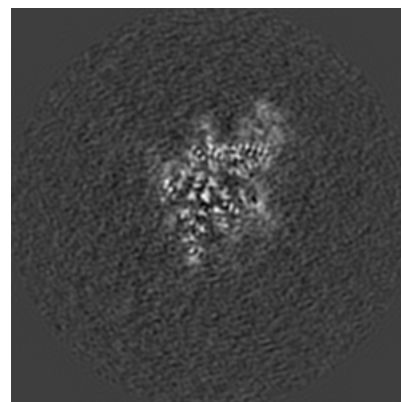
6.2.1 Primary map



X Index: 144



Y Index: 144

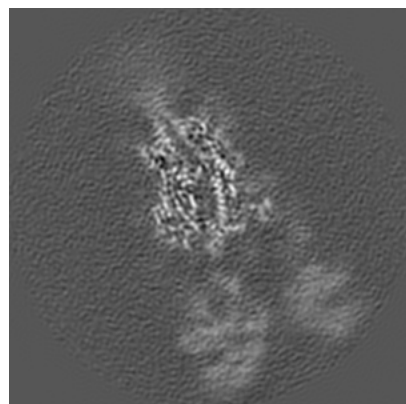


Z Index: 144

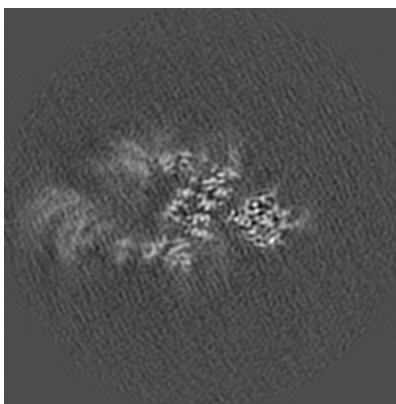
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

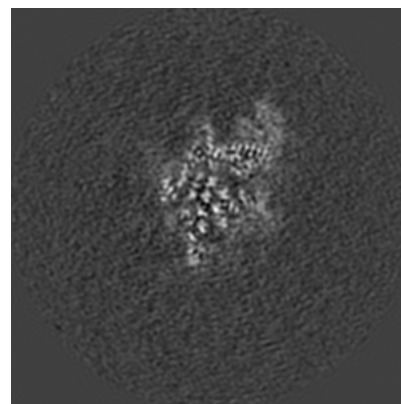
6.3.1 Primary map



X Index: 130



Y Index: 141

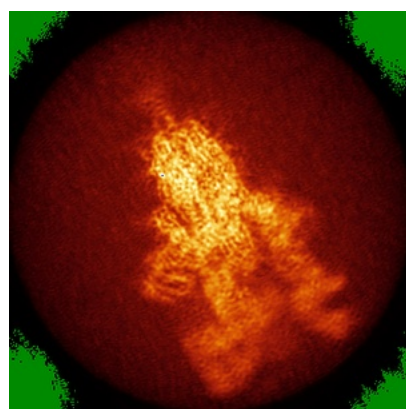


Z Index: 143

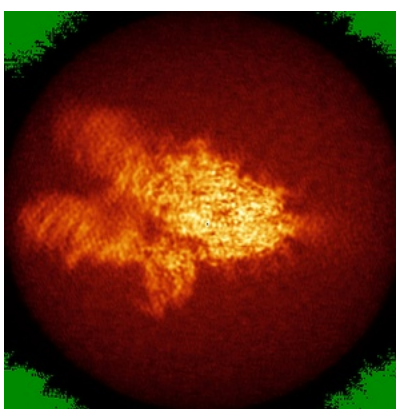
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

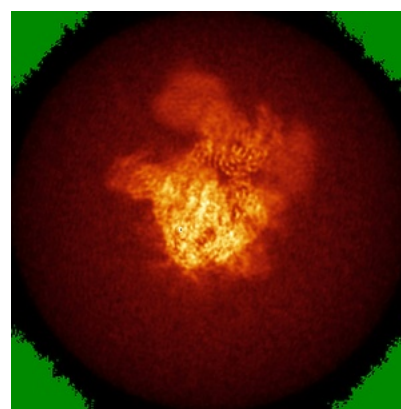
6.4.1 Primary map



X



Y

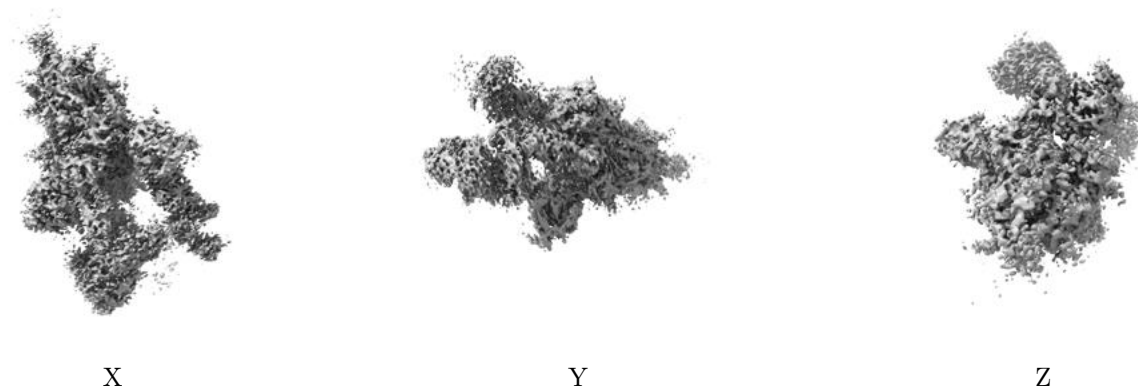


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

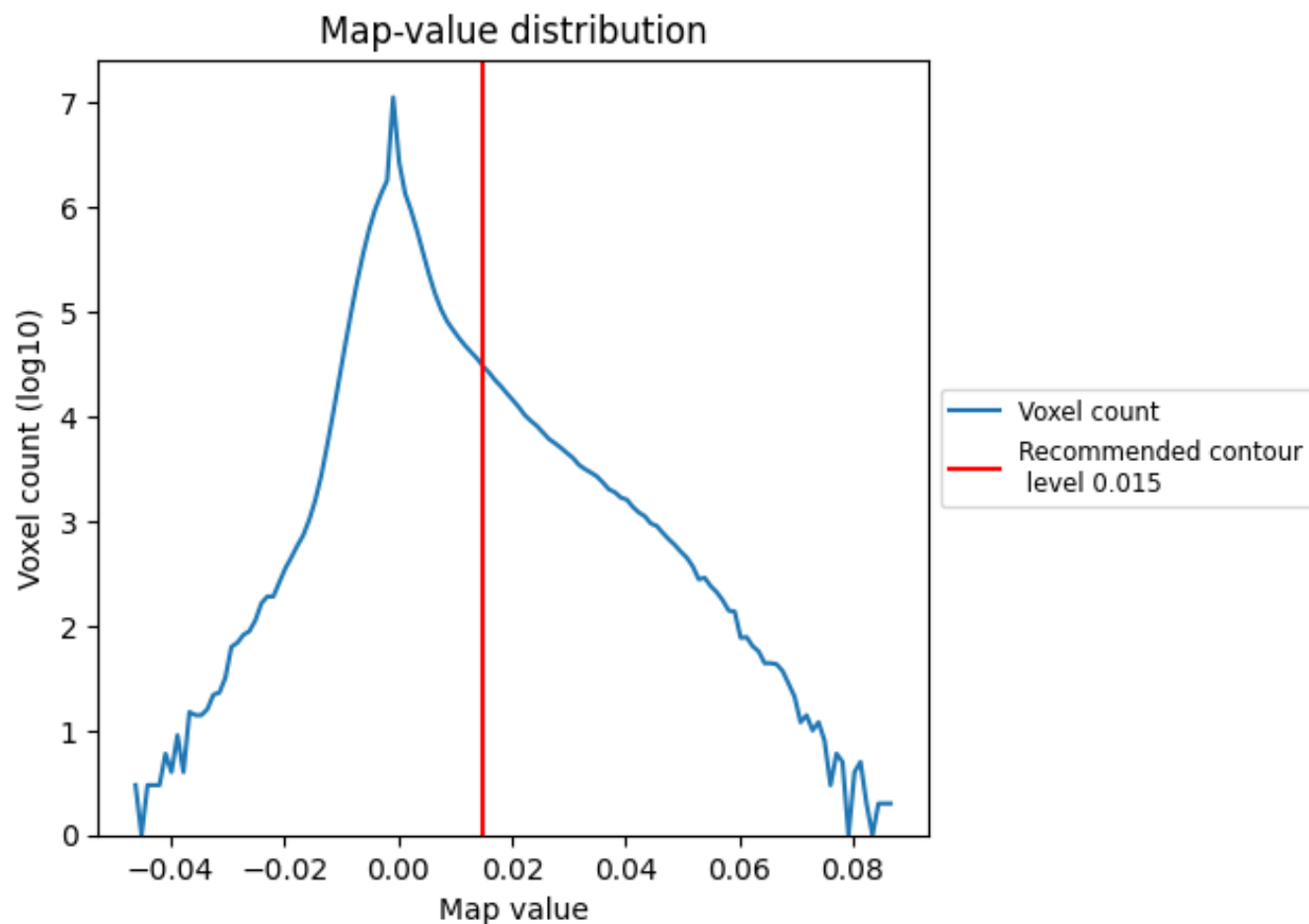
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

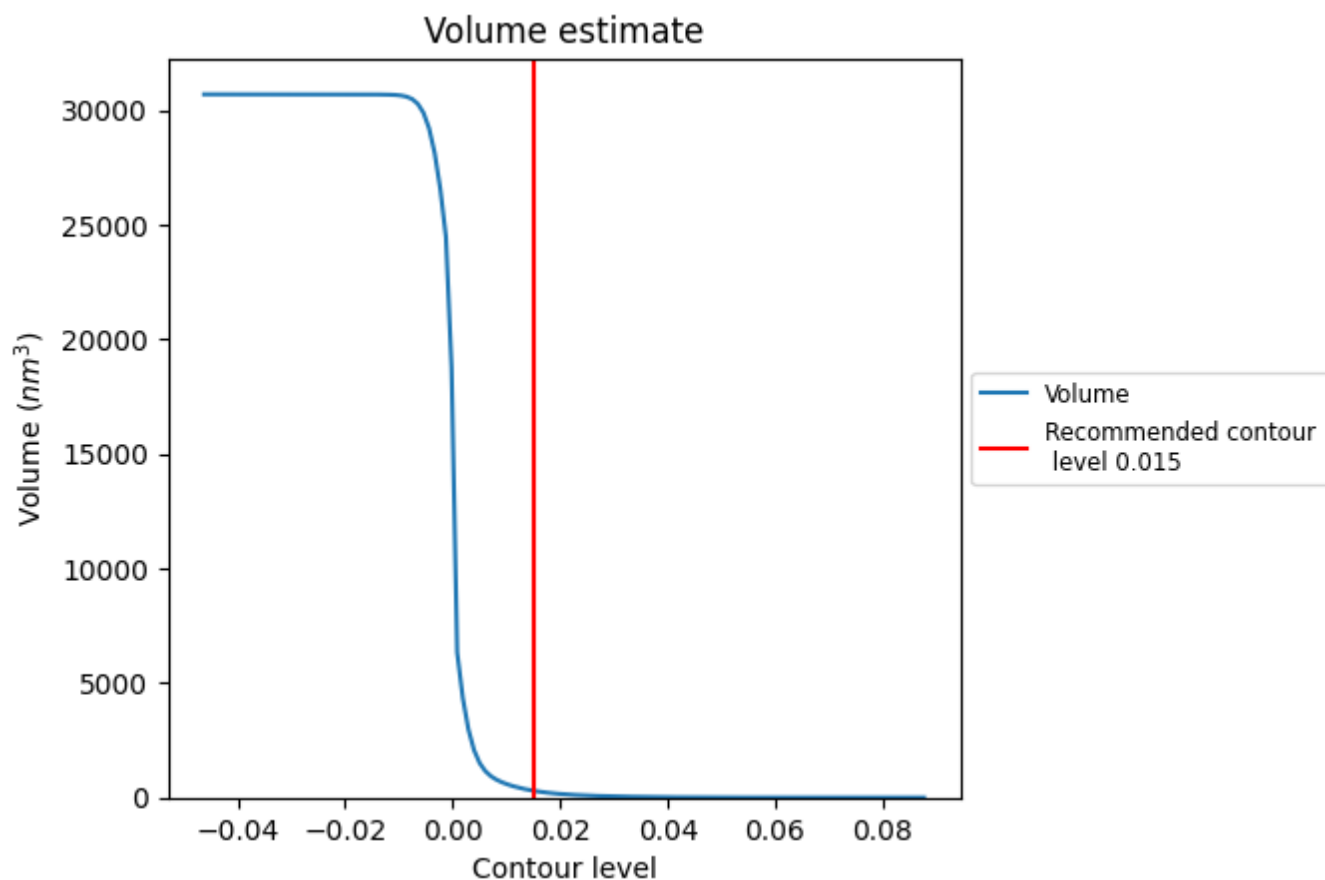
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

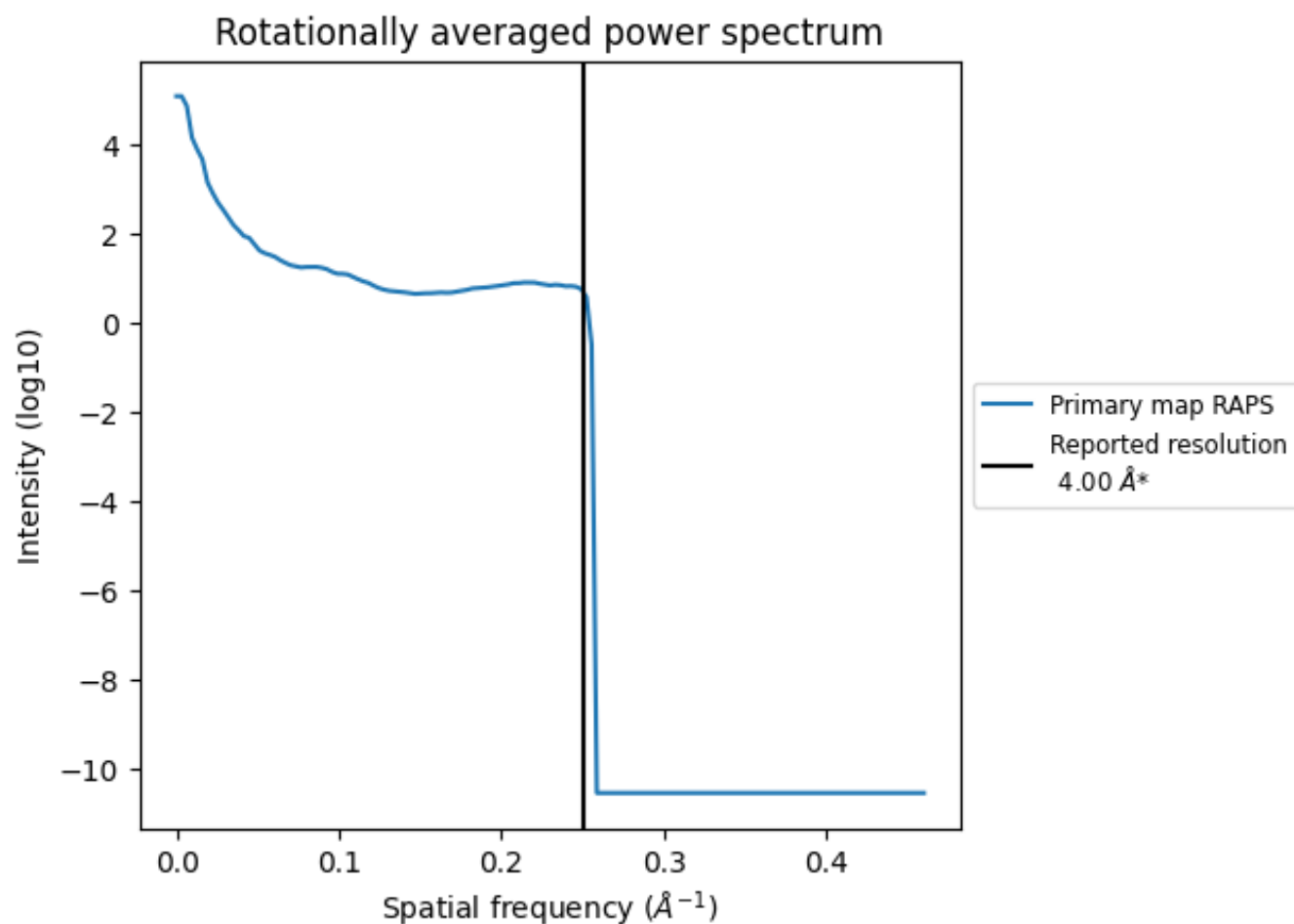
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm³; this corresponds to an approximate mass of 270 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

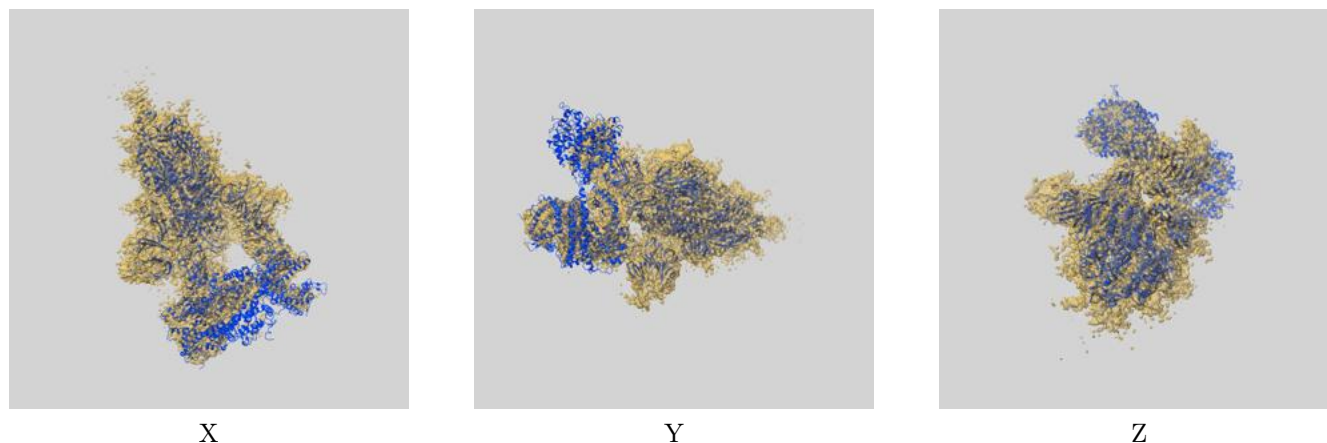
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

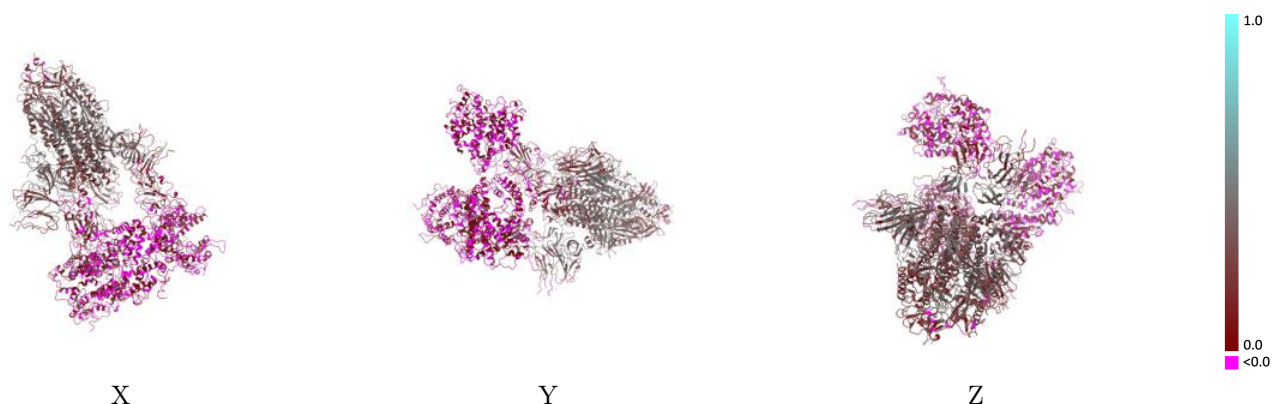
This section contains information regarding the fit between EMDB map EMD-30460 and PDB model 7CT5. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



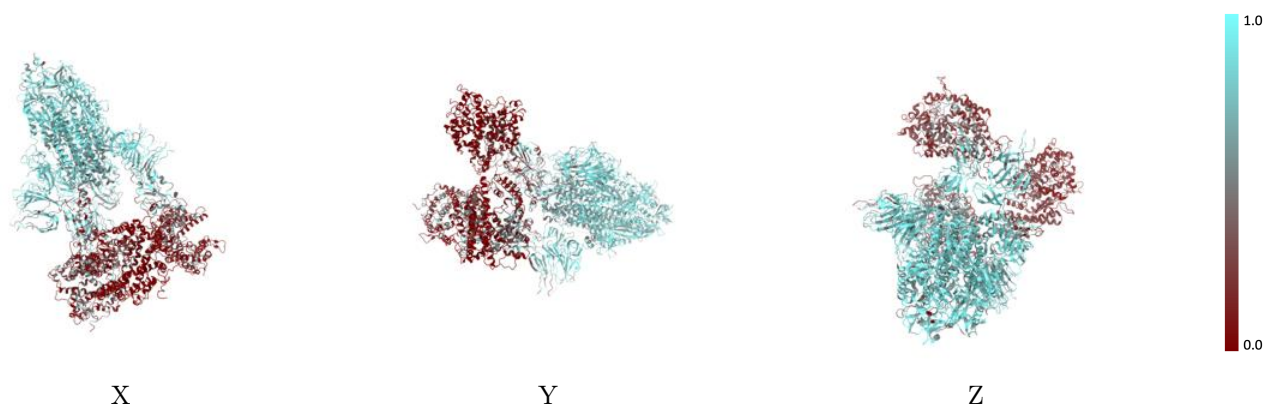
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



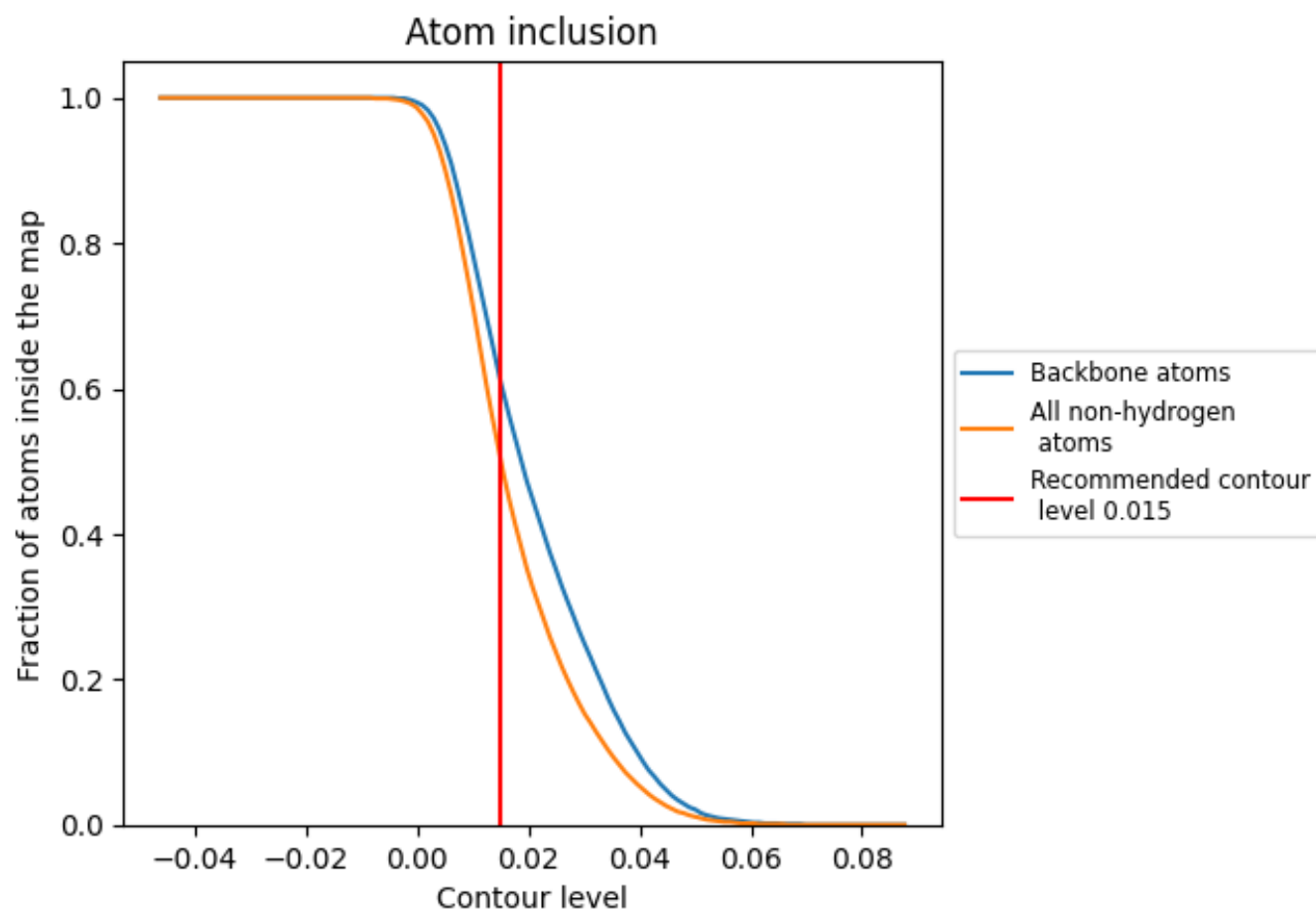
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ















The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5010	 0.1860
A	 0.7000	 0.2650
B	 0.7000	 0.2710
C	 0.7350	 0.2970
D	 0.1480	 0.0320
E	 0.0490	 0.0180
F	 0.2970	 0.0630
G	 0.7140	 0.3250
H	 0.3570	 0.1000
I	 0.7140	 0.3640
J	 0.7140	 0.3390
K	 0.5360	 0.2820
L	 0.7500	 0.2860
M	 0.5710	 0.2910
N	 0.0710	 0.0170
O	 0.4640	 0.2090
P	 0.6070	 0.2600
Q	 0.6790	 0.2600
R	 0.7140	 0.2600
S	 0.7500	 0.3610
T	 0.4640	 0.3000
U	 0.4640	 0.2050
V	 0.6790	 0.3760
W	 0.6430	 0.2440
X	 0.2860	 0.0940
Y	 0.8210	 0.2980
Z	 0.7140	 0.3070
a	 0.0000	 -0.0170
b	 0.0000	 -0.0750
c	 0.0000	 0.0180
d	 0.0000	 0.1300
e	 0.0000	 0.1150
f	 0.0000	 -0.0890
g	 0.0000	 -0.0210
h	 0.0000	 0.1310



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Chain	Atom inclusion	Q-score
i	 0.0000	 -0.0670
j	 0.0000	 0.0730
k	 0.0000	 -0.0600
l	 0.1430	 -0.0620
m	 0.0710	 0.0520
n	 0.0000	 0.1620
o	 0.1070	 0.1620